AN ALTERNATIVES ASSESSMENT FOR THE FLAME RETARDANT DECABROMODIPHENYL ETHER (DecaBDE)

DRAFT FOR PUBLIC COMMENT

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List of Acronyms and Abbreviations

ABS	Acrylonitrile butadiene styrene
ACR	Acute to chronic ratio
ASTM	American Society for Testing and Materials
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BOD	Biochemical oxygen demand
CA - C	Chemical action in condensed phase
CA - G	Chemical action in gas phase
CASRN	Chemical Abstracts Service Registry Number
CDC	Centers for Disease Control and Prevention
CF	Char former
CFR	Code of Federal Regulations
CHO	Chinese hamster ovary cells
ChV	Chronic value
CPE	Chlorinated polyethylene
CPSC	Consumer Product Safety Commission
D	Dilution effect
DecaBDE	Decabromodiphenyl ether
DfE	Design for the Environment
EC_{50}	Half maximal effective concentration
ECHA	European Chemicals Agency
ECOSAR	Ecological Structure Activity Relationships
EDSP	Endocrine Disruptor Screening Program
EEC	European Economic Community
EPA	U.S. Environmental Protection Agency
EPI	Estimations Program Interface
EPDM	Ethylene propylene diene monomer
ERMA	Environmental Risk Management Authority
EU	European Union
EVA	Ethylene vinyl acetate
FAA	Federal Aviation Administration
FM	Factory Mutual
FMVSS	Federal Motor Vehicle Safety Standard
FOB	Functional observational battery
GD	Gestation day
GHS	Globally Harmonized System of Classification and Labeling of Chemicals
GLP	Good Laboratory Practice
HGPRT	Hypoxanthine-guanine phosphoribosyl-transferase
HIPS	High-impact polystyrene
HPLC	High performance liquid chromatography
HPV	High Production Volume
HS	Heat sink
HSDB	Hazardous Substances Data Bank
ICCA	International Council of Chemical Associations

I	Intumescent
IC2	Interstate Chemicals Clearinghouse
ID_{50}	Median ineffective dose
IFR	Inherently flame retardant
IRIS	Integrated Risk Information System
IUCLID	International Uniform Chemical Information Database
K_{oc}	Organic carbon/water partition coefficient (a.k.a. soil adsorption coefficient)
K_{ow}	Octanol/water partition coefficient
LC_{50}	Median lethal concentration
LC_{100}	Absolute lethal concentration
LCA	Life cycle assessment
LCP	Liquid crystal polymer
LD_{50}	Median lethal dose
LD	Lactation day
LFL	Lower limit of flammability
LOAEC	Lowest observed adverse effect concentration
LOAEL	Lowest observed adverse effect level
LOEC	Lowest observed effect concentration
LOEL	Lowest observed effect level
MF	Molecular formula
MITI	Japanese Ministry of International Trade and Industry
MSDS	Material Safety Datasheet
MSP	Mesoporous silicate particle
MW	Molecular weight
NAS	National Academy of Sciences
NCI	National Cancer Institute
NES	No effects at saturation
NFPA	National Fire Protection Association
NGO	Non-governmental organization
NHANES	National Health and Nutrition Examination Survey
NHATS	National Health and Aging Trends Study
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
NOAEC	No observed adverse effect concentration
NOAEL	No observed adverse effect level
NOEC	No observed effect concentration
NOEL	No observed effect level
NTP	National Toxicology Program
OECD	Organisation of Economic Cooperation and Development
OPP	Office of Pesticide Programs
OPPT	Office of Pollution Prevention and Toxics
ORD	Office of Research and Development
PBDE	Polybrominated diphenyl ether
PBT	Polybutylene terephthalate
PBT Profiler	Persistent, Bioaccumulative, and Toxic Chemical Profiler
PA	Polyamide
PC	Polycarbonate

PC-ABS	Polycarbonate-acrylonitrile butadiene styrene
PE	Polyethylene
PET	Polyethylene terephthalate
phr	Parts per hundred of resin
PI	Polyimides
PMN	Premanufacture Notice
PP	Polypropylene
PPE-HIPS	Polyphenylene ether – high-impact polystyrene
ppm	parts per million
PS	Polystyrene
PVC	Polyvinyl chloride
QSAR	Quantitative Structure Activity Relationships
REACH	**R**egistration, **E**valuation, **A**uthorisation and Restriction of **Ch**emical substances
RoHS	Restriction of Hazardous Substances
SAR	Structure Activity Relationship
SF	Sustainable Futures
SIDS	Screening Information Data Set
SMILES	Simplified Molecular-Input Line-Entry System
SPARC	Sparc Performs Automated Reasoning in Chemistry
SVHC	Substance of Very High Concern
TB	Technical Bulletin
TL_{50}	Median tolerance limit
TPU	Thermoplastic polyurethane
TRI	Toxics Release Inventory
TSCA	Toxic Substances Control Act
TSO	Technical Standard Order
UCLA	University of California, Los Angeles
UFL	Upper limit of flammability
UL	Underwriters Laboratory
UPE	Unsaturated polyester
VCCEP	Voluntary Children's Chemical Evaluation Program

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1 Introduction

1.1 Background

As part of its effort to enhance the Agency's current chemicals management program, EPA has taken steps to identify chemicals that may pose environmental and health concerns; in 2009-2011 EPA developed action plans to investigate potential regulatory and voluntary actions. In December 2009, EPA released the Polybrominated Diphenyl Ethers (PBDEs) Action Plan[1] that summarizes hazard, exposure, and use information for three commercial PBDE mixtures, including decabromodiphenyl ether (decaBDE). DecaBDE is a flame retardant used in a variety of applications, including textiles, plastics, wiring insulation, and building and construction materials.

As described in the Action Plan, EPA's Design for the Environment (DfE) Program initiated this multi-stakeholder partnership alternatives assessment: *Flame Retardant Alternatives for Decabromodiphenyl Ether (decaBDE).* DfE's partnerships provide a basis for informed decision-making by developing an in-depth comparison of potential human health and environmental impacts of chemical alternatives. The DfE Alternatives Assessment reports provide information of interest to a number of stakeholder groups interested in chemical hazards. As part of the partnership on flame retardant alternatives to decaBDE, representatives from industry, academia, federal and state governments, and non-governmental organizations (NGOs) engaged with DfE to select and evaluate flame retardant alternatives to decaBDE and develop this report. This report is intended to provide information that will enable the selection of safer alternatives to decaBDE, for a variety of products.

DecaBDE has been used at high volume in a broad range of products, but is now being phased out in the U.S. by its manufacturers (U.S. EPA 2010b). The use of decaBDE was restricted in particular electrical and electronic equipment under the European Union Restriction of Hazardous Substances Directive, with some exemptions (Council of the European Union 2003; Council of the European Union 2011). Additionally, in the U.S., the states of Maine, Maryland, Oregon, Vermont, and Washington have imposed restrictions on the manufacture and/or use of decaBDE in certain applications (Washington 2006; Oregon Legislative Assembly 2009; Vermont 2009; Maine 2010; Maryland 2010). Some additional states have proposed legislation restricting the manufacture and/or use of decaBDE; up-to-date information on state regulations can be found in the U.S. State-level Chemicals Policy Database maintained by the Lowell Center for Sustainable Production: http://www.chemicalspolicy.org/chemicalspolicy.us.state.database.php (Lowell Center for Sustainable Production: University of Massachusetts Lowell 2012). In the private sector, the retailer Wal-Mart has reported that they banned the purchase of all consumer products containing PBDEs, including decaBDE, from their suppliers (Layton 2011).

[1] The Polybrominated Diphenyl Ethers (PBDEs) Action Plan is available online at: http://www.epa.gov/opptintr/existingchemicals/pubs/pbdes_ap_2009_1230_final.pdf

Through EPA's Voluntary Children's Chemical Evaluation Program (VCCEP)[2], industry-sponsored screening level risk assessments for pentaBDE, octaBDE, and decaBDE were developed to evaluate the potential risks to children and prospective parents from potential PBDE exposures (U.S. EPA 2009a). In August 2005, EPA released its Data Needs Decision documents on PBDEs (U.S. EPA 2009a). For decaBDE, EPA indicated a need to further understand fate and transport of decaBDE in the environment, particularly with respect to the significance of its breakdown products, as this could relate to its risk characterization (U.S. EPA 2005d). The decaBDE data needs were not met by the VCCEP sponsors and decaBDE was subsequently terminated from the VCCEP program (U.S. EPA 2009a). EPA then announced its intention to proceed with a test rule under Toxic Substances Control Act (TSCA) section 4 (U.S. EPA 2009a). Before a test rule could be proposed the main manufacturers or importers volunteered to phase out manufacture, import and sales of decaBDE (U.S. EPA 2009a).

DecaBDE is effective in meeting fire safety standards for plastics and textiles that are used for the manufacture of consumer electronics, appliances, wire and cable insulation, building materials (flooring, wall coverings, and roofing), seating, electronics and paneling for cars, buses and airplanes, and storage and distribution products including plastic shipping pallets. Few potential alternatives to decaBDE are "drop-in" replacements (those that require negligible process changes). Use of alternatives may necessitate additional changes in product formulation or movement to different classes of polymers. As companies that have been using decaBDE in their products prepare for the phase out, this alternatives assessment will be an important resource. The information will help reduce the potential for the unintended consequences that could result if functional, but poorly understood alternatives are chosen.

This alternatives assessment evaluated flame retardant alternatives judged by knowledgeable stakeholders as most likely to be used in applications that previously had been filled by decaBDE. The alternatives included in this assessment are viable[3] and functional but not necessarily preferable. Selection of a chemical for evaluation in the report does not denote environmental preferability. Rather, the report provides information that will help decision makers consider environmental and human health profiles for available alternatives, so that they can choose the safest possible functional alternative. This information focuses on the potential hazard associated with a particular chemical. This report also presents general information on exposures to flame retardants, life-cycle considerations, and economic, performance, and social factors.

Assessments of alternatives to decaBDE have been conducted by several organizations in the past, including the Swedish Chemicals Inspectorate, European Commission, Danish Ministry of the Environment, State of Illinois, State of Washington, Clean Production Action, and the University of Massachusetts at Lowell (Pure Strategies Inc. for the Lowell Center for Sustainable Production 2005; Illinois Environmental Protection Agency 2006; Clean Production Action 2007; Danish Ministry of the Environment 2007; European Chemicals Bureau 2007; Washington State Department of Health 2008; Pure Strategies Inc. for Maine Department of Environmental Protection 2010). These assessments looked at decaBDE in a range of applications including

[2] Information on VCCEP is available at: http://www.epa.gov/oppt/vccep.
[3] Viability refers to the functional performance of a chemical as a flame retardant in certain plastics, not the environmental preferability of the chemical nor other product performance criteria.

television enclosures, other electrical and electronic equipment, textiles, residential upholstered furniture and plastics. A few of the studies acknowledged a lack of key information on a number of chemicals, which prevented them from conducting a full hazard assessment of the potential alternatives. In this alternatives assessment report, DfE filled gaps with modeled data estimations and expert judgment, and included assessment of new-to-market decaBDE alternatives.

1.2 Purpose of the Flame-Retardant Alternatives Assessment

The purpose of this alternatives assessment is to identify functional and viable alternatives for decaBDE, evaluate their human health and environmental profiles, and inform decision makers in order for organizations to choose safer alternatives to decaBDE.

1.3 Scope of the Flame-Retardant Alternatives Assessment

The partnership refined the scope of this assessment from the PBDEs Action Plan with information supplied by experts in industries that use decaBDE in their products and from academics, NGOs and government participants. The assessment provides hazard information (human toxicity, ecotoxicity and environmental fate) on flame retardants that were selected for evaluation in this report as potentially functional alternatives to decaBDE. While this project is not designed to recommend specific flame retardants, it does evaluate potential alternatives to decaBDE that have the potential to be functional and viable in certain applications. Therefore, this evaluation can support informed substitution and has the potential to identify environmentally preferable substitutes.

The partnership on flame retardant alternatives to decaBDE is an assessment of hazards of flame retardant chemicals that are potentially functional and viable[3] alternatives to decaBDE. These alternatives have the potential to enable a product to meet relevant flammability standards when used in one or more of the material classes listed below. These materials include those in which decaBDE is currently used or was used in the past. Additionally, polycarbonate and polycarbonate-acrylonitrile butadiene styrene were included because they can be used with some of the alternative flame retardants. The material types that are most relevant to this project include:

1. Polyolefins
    a. Polypropylene (PP)
    b. Polyethylene (PE)
    c. Ethylene vinyl acetate (EVA)

2. Styrenics
    a. High-impact polystyrene (HIPS)
    b. Acrylonitrile butadiene styrene (ABS)

3. Engineering thermoplastics
    a. Polyesters
        i. Polybutylene terephthalate (PBT)
        ii. Polyethylene terephthalate (PET)
    b. Polyamides (PA), e.g., nylon

   c. Polycarbonate (PC) and polycarbonate blends, e.g., polycarbonate-acrylonitrile butadiene styrene (PC-ABS)
   d. Polyphenylene ether – high-impact polystyrene (PPE-HIPS)

4. Thermosets
   a. Unsaturated polyesters (UPE)
   b. Epoxies (electronics, building and aerospace applications)
   c. Melamine-based resins

5. Elastomers
   a. Ethylene propylene diene monomer (EPDM) rubber
   b. Thermoplastic polyurethanes (TPUs)
   c. EVA

6. Waterborne emulsions and coatings – including but not limited to those designed for textile back coatings such as:
   a. Acrylic emulsions
   b. Polyvinyl chloride (PVC) emulsions
   c. Ethylene vinyl chloride emulsions
   d. Urethane emulsions

The scope was outlined in terms of categories of materials rather than specific applications or end-use products because decaBDE has many varied applications. In this approach, the partnership intended to provide toxicity and environmental fate information on potential flame retardant alternatives for product manufacturers who must make substitution decisions, as well as for other interested or affected parties (e.g., end users, downstream processors).

The alternative flame retardant chemicals[4] will be evaluated for hazard potential independent of the materials in which they might be used or incorporated. While the assessment will not attempt to include comprehensive life cycle assessment (LCA) information, it will, by both inclusion and by reference, note relevant life-cycle considerations that may aid in the selection of alternatives. Due to these constraints, this assessment does not provide all of the information that a decision maker may need to be able to choose an alternative flame retardant.

The report is organized as follows:

- *Chapter 1 (Introduction):* This chapter provides background on the Partnership on Flame Retardant Alternatives to decaBDE project, including the purpose and scope of the partnership and of this report.

- *Chapter 2 (Products and Materials):* This chapter describes the products and materials in which decaBDE has been used, as well as technical information about flammability standards and other performance criteria.

[4] For the purposes of this report, 'chemicals' include both discrete substances that can be represented by a definite structural diagram (such as methane) and reaction mixtures that cannot. Reaction mixtures include those that are well defined with a few components (such as propylene glycol), mixtures that may be difficult to characterize and/or are of variable composition (such as polychlorinated biphenyls or Aroclors), and polymers.

- *Chapter 3 (Background on Flame Retardants):* This chapter describes chemical flame retardants generally, as well as those specific to this assessment.

- *Chapter 4 (Evaluation of Flame Retardants):* This chapter explains the chemical assessment method used in this report and summarizes the assessment of hazards associated with each flame retardant chemical.

- *Chapter 5 (General Exposure Information and Life Cycle Considerations):* This chapter includes potential exposure pathways associated with flame retardants along each stage of their life-cycle and resources for life cycle impact information that decision makers may need.

- *Chapter 6 (Considerations for Selecting Flame Retardants):* This chapter identifies human health, environmental, economic, performance and social considerations for selecting alternative flame retardants.

1.4 Chemical Alternatives Assessment as a Risk Management Tool

Among other actions, the Agency chose to conduct an alternatives assessment as a suitable risk management tool for decaBDE in the PBDEs Action Plan. The Agency chose this tool to inform the chemical substitution that may occur as an outcome of other activities described in the Action Plan. Chemical alternatives assessments provide information on the environmental and human health profiles of chemicals that may be used as substitutes so that industry and other stakeholders can use this information, in combination with analyses of cost, performance, and other factors to choose alternatives.

Chemical alternatives assessment, LCA, and risk assessment are all tools that can be used to improve the sustainability profiles of chemicals and products. These tools, which can be complementary, should be selected according to the ultimate action they are intended to support and other regulatory and policy considerations. DfE alternatives assessments establish a foundation that other tools, such as risk assessment and LCA, can build upon.

The focus of this DfE alternatives assessment report is a comparative hazard assessment of the chemical alternatives that may be substituted for decaBDE in a variety of uses. Comparative chemical hazard assessment is a comparison of chemicals within the same functional use group (e.g., solvent, surfactant, flame retardant, ink developer) that evaluates alternatives across a consistent and comprehensive set of hazard endpoints. Information about chemical hazards derived from this type of comparative chemical hazard assessment can be used by decision-makers to help them select safer alternative chemicals.

Risk assessment and alternatives assessment are both based on the premise that risk is a function of hazard and exposure. Risk assessment characterizes the nature and magnitude of hazard and exposure from chemical contaminants and other stressors. The DfE alternatives assessment evaluates and compares the nature of the chemical hazards and reflects a view that when exposure is comparable, risk is reduced through the use of less hazardous chemicals. Alternatives

assessment strives to decrease the reliance on exposure controls thus reducing risk even when exposure controls fail.

Chemical alternatives assessment differs substantially from LCA. An LCA can present a robust picture of many environmental impacts associated with the material and energy inputs and outputs throughout the life cycle of a product, and by doing so can identify opportunities for reducing those impacts. However, unlike chemical alternatives assessment, LCA typically provides a limited (if any) review of inherent toxicity.

DfE's 'functional use' approach to alternatives assessment orients chemical evaluations within a given product type and functionality. Under this approach, factors related to *exposure scenarios*, such as physical form and route of exposure, can be constant within a given functional use analysis and will fall out of the comparison so that a reduction in hazard is a reduction of risk. When less hazardous alternatives have different physical-chemical profiles or require different use levels, it may be appropriate to also conduct an exposure assessment. DfE alternatives assessments consider intrinsic properties of chemical substitutes that affect *exposure potential*, including absorption potential, persistence, and bioaccumulation. Under this approach, the health and environmental hazard profiles in the alternatives assessments become the key variable and source of distinguishing characteristics. Information on key properties that can be used to evaluate significant differences in environmental fate and transport, including persistence, bioaccumulation, and physical properties, are included in Chapters 4 and 5.

Chemical alternatives assessment is most useful in identifying safer substitutes when available alternatives meet performance requirements and are expected to present lower hazards for human health and the environment. During decision-making, risk assessment or LCA could be applied to the lower-hazard or potentially preferable alternatives to complement the alternatives assessment findings. Alternatives assessment can identify scenarios in which initial comparisons indicate that there may be no preferable alternatives to the chemical being considered. However, this can guide innovation and product development by understanding the characteristics of a safer alternative.

The DfE chemical alternatives assessment approach is aligned with green chemistry principles[5]. Two of those principles are especially noteworthy:

- Principle 4: Design of safer chemicals – "Chemical products should be designed to effect their desired function while minimizing their toxicity," and

- Principle 10: Design for degradability – "Chemical products should be designed so that at the end of their function they break down into innocuous degradation products and do not persist in the environment."

DfE incorporates these two green chemistry principles in its criteria and applies them in its assessment of chemical hazard and fate in the environment. This approach enables identification of safer substitutes that emphasize greener chemistry and points the way to innovation in safer chemical design where hazard becomes a part of a performance evaluation.

[5] http://www.epa.gov/sciencematters/june2011/principles.htm

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2 Products and Materials

DecaBDE is used for fire safety in a broad range of plastics and polymers with product applications in diverse sectors. Presented below are the categories of materials (Section 2.1) and sectors and products (Section 2.2) for which decaBDE has been or is currently used. Flammability standards relevant for products containing decaBDE are discussed briefly at the end of the chapter (Section 2.3).

2.1 Materials Outlined in the Scope

The materials included in this section are those in which decaBDE is currently or was used in the past. Additionally, polycarbonate (PC) and polycarbonate-acrylonitrile butadiene styrene (PC-ABS) were included because they can be used with some of the alternative flame retardants. These materials are polymers, made up of chains of repeating monomer units. Table 2-1 displays end-uses by polymer group, each of which may contain several different polymers. A key characteristic of these polymers is whether or not they can be reprocessed and therefore this is touched on in each section. The end-use products and sectors for these materials are discussed in Section 2.2. DecaBDE may not be used in all polymer/end-use application combinations; those relevant to decaBDE are noted in Section 2.2.

Table 2-1: Summary of Polymers and Their End-Use Application

Polymer Group	End-Use Applications								
	Electronics	Wire and Cable	Public Buildings	Construction Materials	Automotive	Aviation	Storage and Distribution Products	Textiles	Waterborne emulsions & coatings
Polyolefins	✓	✓	✓	✓	✓	✓	✓	✓	✓
Styrenics	✓		✓	✓	✓	✓	✓		
Engineering Thermoplastics	✓	✓	✓	✓	✓	✓		✓	✓
Thermosets	✓		✓	✓	✓	✓	✓	✓	✓
Elastomers	✓	✓	✓	✓	✓	✓	✓	✓	✓
Waterborne emulsions and coatings[1]	✓	✓	✓	✓	✓			✓	✓

[1] Includes acrylic, polyvinyl chloride (PVC), ethylene vinyl chloride, and urethane emulsions

Source: Personal communication with members of the partnership

2.1.1 Polyolefins

There are a variety of polyolefins but only three in which decaBDE is commonly used: polypropylene (PP), which has the molecular formula $(C_3H_6)_n$; polyethylene (PE), which has the molecular formula $(C_2H_4)_n$; and ethylene vinyl acetate (EVA)[6], which is a copolymer of ethylene and vinyl acetate, $(C_2H_4)_m$ $(C_4H_6O_2)_n$ (Mark 2009). Polyolefins are polymers with single carbon bonds, but are derived from hydrocarbons with carbon-carbon double bonds (e.g., ethylene). The basic repeating unit has the molecular formula of C_nH_{2n}. Polyolefins can soften and eventually melt upon heating. As a result, they can be reprocessed which allows them to be remolded repeatedly (Harper and Modern Plastics 2000; Rex 2011). Polyolefin materials can be flexible and are used for applications such as garbage bags, undergarments for wet suits, foam shoes, seat cushions, arm rests, shrink film, and other products (Mark 2009). Additional important polyolefins applications include wire and cable, electrical connectors, battery casings, foamed sheets and pipes for thermal insulations.

2.1.2 Styrenics

Styrenics are based on styrene monomers, also known as vinyl benzene, which consist of a phenyl group attached to a two-carbon chain, $CH_2=CH(C_6H_5)$. There are several different types of styrene plastics, two of which can contain decaBDE: high-impact polystyrene (HIPS) and acrylonitrile butadiene styrene (ABS). Polystyrene (PS) and styrene copolymers tend to be brittle, so rubber particles are added to increase impact resistance (Howe-Grant 1997a; Rex 2011). Like polyolefins, styrenics can soften and eventually melt upon heating. As a result, they can also be reprocessed which allows them to be remolded repeatedly (Harper and Modern Plastics 2000; Rex 2011). The following descriptions provide an overview of each material and its general application.

> *HIPS*. HIPS is produced by combining PS with rubber particles, which gives it the mechanical properties that make it suitable for use in durable molded items. Its historical use in television casings is a well-known example (Harper and Modern Plastics 2000).
>
> *ABS*. ABS is a mixture of acrylonitrile, butadiene, and styrene. In general, ABS is widely used in the casing of equipment for telephones, televisions, and computers (Harper and Modern Plastics 2000).

2.1.3 Engineering Thermoplastics

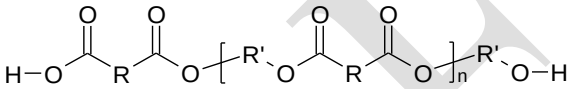
Engineering thermoplastics are materials that are typically not cross-linked, can soften and eventually melt upon heating, and have high levels of mechanical and thermal performance in molded goods when compared to commodity thermoplastics (e.g., PP, PE, HIPS, etc.). As a result, thermoplastics can be reprocessed (Harper and Modern Plastics 2000). This property of thermoplastics allows them to be remolded repeatedly. There are several types of engineering thermoplastics in which decaBDE can be used, including polyester, polyamide (PA), PC, and

[6] EVA is a copolymer of ethylene (an olefin) and vinyl acetate, therefore it is considered to be a polyolefin. However, EVA also has elastomeric properties. For this reason, this report classifies EVA as both a polyolefin and an elastomer. For further discussion on EVA, see Section 2.1.5 on elastomers.

polyethylene ether – high-impact polystyrene (PPE-HIPS). The following descriptions provide an overview of each material and their general applications.

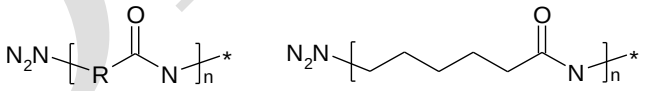
Polyesters. Polyesters (see Figure 2-1) are a broad class of thermoplastics characterized by an ester linkage. Within this class, decaBDE can be used in polybutylene terephthalate (PBT) and polyethylene terephthalate (PET). The only structural difference between PBT and PET is the presence of four methylene repeat units in each PBT repeat unit rather than the two present in each PET repeat unit. PBT has numerous automotive applications such as the exterior as well as connectors for under-the-hood electronic controls. Another major use of PBT is in glass-reinforced grades that are often in switches and connectors for electrical equipment. PET has many commercial applications in injection moldings, blow-molded bottles, and films (Harper and Modern Plastics 2000). Polyesters are also used in commercial and domestic carpeting and textile fibers.

Figure 2-1: Chemical Structure of Polyester



PAs. PAs (see Figure 2-2), also referred to as nylons, are characterized by amide groups along the polymer backbones. There are several types of PAs, the majority of which are used in injection molding applications in information technologies and the transportation industry, mostly for automobiles. PAs are used in automobile exteriors (e.g., wheel covers and handles), interiors (e.g., chair and seat belt mechanisms and light housings), under-the-hood applications, and commercial and domestic carpeting and textile fibers (Howe-Grant 1997d). Glass-reinforced grades also use PAs in electrical switches and connectors.

Figure 2-2: Chemical Structure of PA and Nylon

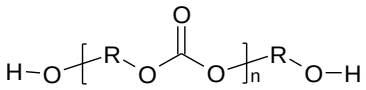


PA Nylon

PCs. PCs (see Figure 2-3) contain a carbonate group and have an excellent combination of mechanical properties, which make them ideal for a variety of applications. PC is a good choice for applications requiring higher use temperatures, lower flammability, and greater impact strength, assuming that the application can afford the higher cost of PC. They are commonly used to manufacture roofing panels, windows for aircraft, trains, and schools, and to make automotive components, such as headlamps and bumpers. Additionally, PC is used to make plastic bottles, CDs & DVDs, electrical equipment, especially connectors, and motorcycle and football helmets. PC is also commonly blended with other materials, such as ABS, to achieve lower cost and improved

properties (Howe-Grant 1997e). For example, sometimes PC is added to polymers to impart improved thermal deflection properties. PC-ABS blends are used for equipment housing and structural parts that require high levels of stiffness, gloss, and impact resistance (Weil and Levchik 2009).

Figure 2-3: Chemical Structure of PC



PPE-HIPS. PPE-HIPS, a polymer blend, imparts a higher heat resistance compared to PS. PPE-HIPS is commonly used for dishwashers, washing machines, hair dryers, cameras, instrument housings, and in television accessories (Harper and Modern Plastics 2000).

2.1.4 Thermosets

Thermosets (also referred to as 'thermoset plastics') undergo an irreversible chemical cross-linking reaction upon curing. Unlike styrenics, polyolefins and thermoplastics, thermosets cannot be reprocessed once they cure/polymerize; they are insoluble in most solvents and can only be broken up by breaking chemical bonds (Mark 2009). While the inability to reprocess thermosets presents some drawbacks, it also gives thermoset plastics enhanced properties that are maintained in extreme conditions (Harper and Modern Plastics 2000). There are several types of thermosets in which decaBDE can be used, including unsaturated polyesters (UPEs), epoxies, and melamine-based resins. The following descriptions provide an overview of each material and their general applications.

UPE. UPEs are produced from maleic anhydrides and alcohols, and are used to produce molding compounds. UPEs contain an unsaturated diacid (typically maleic acid or fumaric acid) which can be cross-linked during the curing process; additionally a reactive solvent/monomer is also added before curing (American Composites Manufacturers Association 2004). Other acids and alcohols are added for desired chemical properties. Typical applications include automotive and building components, commercial connectors, and various household articles (Harper and Modern Plastics 2000; Troitzsch 2004).

Epoxies. Epoxies are co-polymers formed from the reaction of two chemicals: a resin that consists of a short chain polymer with epoxy groupings at either end, and a hardening or cross linking agent. The reaction forms a three-dimensional lattice. These epoxies have excellent adhesion properties as well as chemical and heat resistance. As a result, they can be used in thermal insulation as well as in electronics (Mark 2009). Epoxies are used broadly, from high-performance military to commodity commercial applications, such as connectors, relays, printed circuit boards, switches, coils, aircraft skins, and satellite parts (Harper and Modern Plastics 2000).

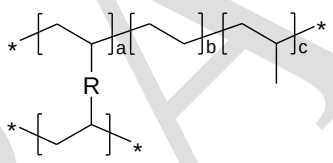
Melamine-Based Resins. Melamine-based resins are a type of amino resin made by combining melamine ($C_3H_6N_6$) with formaldehyde (CH_2O). Melamine-based resins are used as textile-finishing materials to provide wash-and-wear properties to cellulosic fabrics (Howe-Grant 1997b).

2.1.5 Elastomers

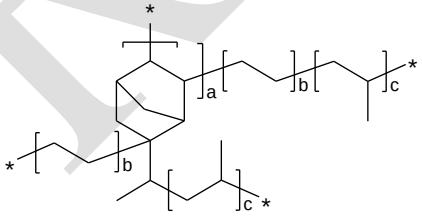
Elastomers are rubberlike materials that can recover their original shape after being stretched or compressed (Howe-Grant 1997c). There are three types of elastomers in which decaBDE can be used: (1) ethylene propylene diene monomer (EPDM) rubber, (2) thermoplastic polyurethanes (TPUs), and (3) EVA[7]. The following descriptions provide an overview of each material and their general applications.

EPDM. EPDM (see Figure 2-4) is a copolymer of ethylene, propylene, and a diene, and is mainly used in automotive applications as radiator hoses and seals; in building and construction as roofing membranes and pond liners; in cable and wire as insulation and jacketing; and in appliances as molded components (Howe-Grant 1997c; Ciesielski 2000).

Figure 2-4: Chemical Structure of EPDM Polymer



EPDM



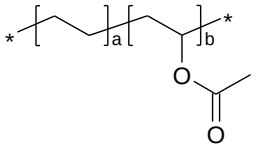
Common Example of EPDM.
Note: "a" is small compared to "b" and "c".

TPUs. TPUs contain carbamate groups, also referred to as urethane groups, in their backbone structure (Howe-Grant 1997f). The mechanical properties of TPUs fall between rubber polymers and thermoplastics, and they are made into products through injection or extrusion. TPUs have a variety of uses in automobiles, as well as in medical equipment, wire and cable, and other applications (Randall 2010).

[7] EVA is a copolymer of ethylene (an olefin) and vinyl acetate, therefore it is considered to be a polyolefin. However, EVA also has elastomeric properties. For this reason, this report classifies EVA as both a polyolefin and an elastomer.

EVA. EVA (see Figure 2-5) is typically used in 'hot-melt' formulations. EVA based hot-melts have various applications, such as packaging, bookbinding and labeling (SpecialChem 2011).

Figure 2-5: Chemical Structure of EVA



2.1.6 Waterborne Emulsions and Coatings

There are three types of waterborne emulsions and coatings in which decaBDE can be used: acrylic, PVC and ethylene vinyl chloride, and urethane. The following descriptions provide an overview of each material and their general applications.

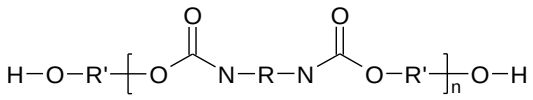
Acrylic. Acrylic emulsions are aqueous, anionic, emulsion-polymerized dispersions of acrylate copolymers. According to a manufacturer website, acrylic emulsions are used for their heat sealability, resistance to heat and light discoloration, good initial color and clarity, and overall durability (Lubrizol 2011). Acrylic emulsions may fade over time, depending on the quality of the colorants or pigments used (Jones 2004; Smithsonian Institution 2011). Acrylic emulsions span a wide range of polymer and end-use properties. While acrylic emulsions are frequently used in nonwoven and paper saturation applications, many are equally applicable for paint and coatings applications. These formulations can be molded into very soft, flexible coatings or very hard, stiff coatings (Friddle 2011).

PVC and Ethylene Vinyl Chloride. Vinyl chloride emulsions are aqueous anionic dispersions of vinyl chloride and copolymers. These emulsions are primarily designed for coating, impregnation and saturation of fibrous materials such as paper, nonwovens and textiles. Their heat reactive nature poses excellent adhesion to various substrates, and they are commonly used in wall covering and resilient flooring (Friddle 2011).

Vinyl chloride polymers are used in textile coatings, nonwovens, paper, paints, and graphic arts applications. Ethylene vinyl chloride polymers are used in a variety of adhesive applications, such as paper packaging, wood bonding, furniture, book binding, wall and ceiling coverings, flooring, consumer glues, and film laminates (Friddle 2011).

Urethane. Polyurethanes (see Figure 2-6) are the most well-known polymers used to make foams, though they can also be elastomers. Polyurethane materials are commonly formulated as paints or finishing coats to protect or seal wood and textiles (Friddle 2011).

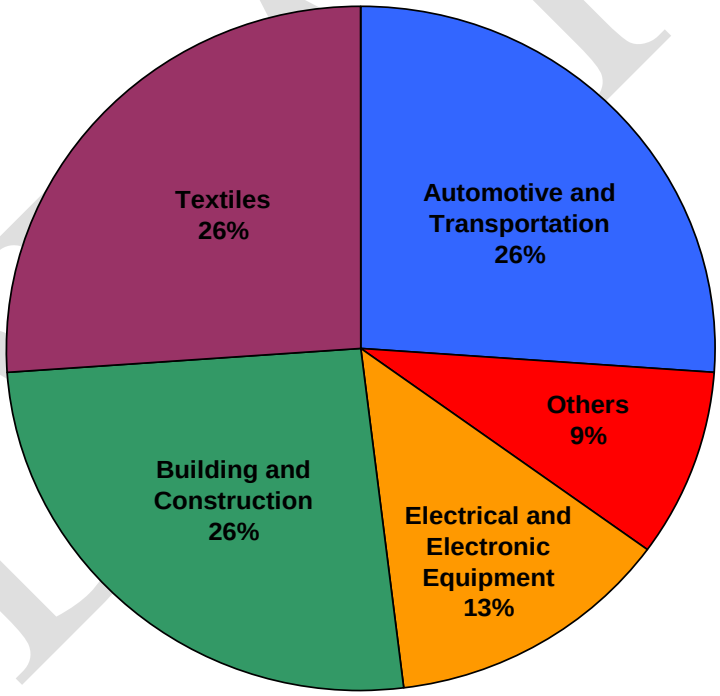
Figure 2-6: Chemical Structure of Polyurethane



2.2 Uses of decaBDE

The purpose of this section is to highlight the various uses of decaBDE. The profile of industries and products using decaBDE has changed in recent years, mainly due to changing international and state-based regulation. A current estimate of the use profile for decaBDE is represented in Figure 2-7. For information on exposure to flame retardants due to the use of these products see Chapter 5.

Figure 2-7: Segmentation of decaBDE Uses, by weight, in the USA[1]



[1] Imports of manufactured goods are not included in the chart.
Source: Levchik 2010

Many electronics manufacturers have moved away from using decaBDE in HIPS, especially in Europe, where the Restriction of Hazardous Substances (RoHS) Directive has banned the use of decaBDE in electronics (Council of the European Union 2003; Washington State Department of

Health 2008; Council of the European Union 2011); with certain exemptions. A use profile such as the one shown in Figure 2-7 for previous years, prior to RoHS, was not available when this report was compiled. However, in 2003 it was estimated that 80 percent of decaBDE was used in electronics (which included television enclosures, central processing unit housing and wire and cable) and 10 to 20 percent of decaBDE was used in textiles (which included upholstered furniture and automotive upholstery) (Hardy 2003). Additionally, although HIPS containing decaBDE was once used in office machines such as printers, copiers, and fax machines, these products are now made using other types of plastics that do not contain decaBDE (Pure Strategies Inc. prepared for the Maine Department of Environmental Protection 2010). Furniture manufacturers are also expected to shift towards barrier technologies (Pure Strategies Inc. prepared for the Maine Department of Environmental Protection 2010). To the best of our knowledge decaBDE was not used in mattresses or polyurethane foam for furniture, but can be used in textile back-coatings for furniture (Trainer 2010). For further information on flame retardants for polyurethane foam, refer to the *Profiles of Chemical Flame-Retardant Alternatives for Low-Density Polyurethane Foam* report (U.S. EPA 2005a).

2.2.1 Electrical and Electronic Equipment

Historically, most decaBDE was used in electrical and electronic equipment in plastic casings, wire and cable and small electrical components to meet fire safety standards (see Table 2-2). The main use of decaBDE was in the front and back panels of televisions made of HIPS (Lowell Center for Sustainable Production 2005). Additionally, decaBDE was often used in electronic connectors made from glass-filled PBT or nylons (Levchik 2010). With the European RoHS Directive, many global companies have phased out decaBDE in these uses.

Box 2-1 DecaBDE is, or has been, used in the following electric and electronic applications:

- Housings and internal components of TVs
- Mobile phones and fax machines
- Audio and video equipment
- Remote controls
- Communications cables
- Capacitor films
- Building cables
- Wire and cable, e.g., heat shrinkable tubes
- Connectors in electrical and electronic equipment
- Circuit breakers
- Coils of bobbins (i.e., for use in transformers)
- Printing and photocopy machine components – e.g., plastic housing for toner cartridges
- Scanner components

Source: Bromine Science and Environmental Forum 2007

Despite this transition, decaBDE is still used in a variety of electronic equipment including household appliances and tools such as vacuum cleaners (in both the casings and internal components) and washing machines (internal components only) because the markets for these products are more domestic than global and European Union regulations have not impacted the use of decaBDE in these products as significantly (Levchik 2010). In these appliances, the housings are typically made from PP, HIPS or ABS.

Another use of decaBDE is in small electrical parts, such as light sockets or decorative lights (e.g., Christmas lights), and wires and cables. These products are usually made from high density PE, PP or PPE (Levchik 2010). DecaBDE is also used in the plastics PBT and PA, which are found in electrical, automotive,

and plumbing parts such as housings, switches and other small inner parts of larger electrical equipment (Weil and Levchik 2009). DecaBDE is also commonly used in electrical components of cars and airplanes, which will be discussed in Section 2.2.4.

2.2.2 Textiles

Another major use of decaBDE is in textiles. Flame retardants are applied to textiles in order to meet required flammability standards (see Table 2-2). They are often applied to the back of a fabric as part of a coating that also contains antimony trioxide in an acrylic or EVA copolymer (Lowell Center for Sustainable Production 2005).

The uses of decaBDE in textiles for the automotive and aviation sectors are discussed in more detail in Section 2.2.4. DecaBDE is not used in consumer clothing (e.g., children's pajamas) (Pure Strategies Inc. for the Lowell Center for Sustainable Production 2005) or in residential carpet (Levchik 2010). Residential carpet is mainly flame retarded by addition of aluminium hydroxide to the back coating. Children's pajamas often meet flammability standards without the use of flame retardants. This is because children's pajamas need to pass the Consumer Product Safety Commission (CPSC) ignition test (three seconds of flame exposure), which can be passed by synthetic fabrics without addition of any flame retardant (Levchik 2010).

Box 2-2 DecaBDE is or has been used in the following textile applications:

- Transportation
  - Public transit busses
  - Trains
  - Airplanes
  - Ships
- Public occupancy spaces
  - Draperies of theatres, hotels, conference rooms, student dormitories
- High-risk occupancy areas
  - Furniture of nursing homes, hospitals, prisons, hotels
- Military
  - Tarps
  - Tents
  - Protective clothing

Source: Bromine Science and Environmental Forum 2007

Box 2-3 DecaBDE is used in the following building and construction applications:

- Pipes
- Lamp holders
- Stadium seats
- Reinforced plastics
- Switches and connectors
- Facing laminates for insulation panel
- Film for use under the roof and to protect building areas
- Electrical ducts and fittings
- Components in analytical equipment in industrial
- Medical laboratories
- Air ducts for ventilation systems
- Pillars for telephone and communication cables

Source: Bromine Science and Environmental Forum 2007

2.2.3 Building and Construction

DecaBDE is used in wall and roof panels, which are typically made from UPE glass composites; floor tiles; and commercial grade carpeting. DecaBDE is also used in insulation materials, foamed polyolefins, and in roofing materials such as membranes and films for use under roofs to protect building areas. DecaBDE can also be found in ducting elements such as the duct covering or insulation.

2.2.4 Transportation

In automobiles, decaBDE is added to plastics used to house and insulate electrical and electronic equipment under the hood. There are no broad federal fire safety standards or regulations for these applications; safety standards are established by each manufacturer. Interior materials, such as cushioning and fabric must meet the Federal Motor Vehicle Safety Standard (FMVSS) No. 302 (U.S. Department of Transportation and National Highway Traffic Safety Administration 1972; Levchik 2010). DecaBDE may also be used in parts of the heating, ventilation, and air conditioning system close to or in contact with electrical parts (Levchik 2010).

In aircraft, decaBDE is used in electrical and electronic equipment (Levchik 2010), and interior components. Materials used on aircraft must meet Federal Aviation Administration (FAA 2010) Technical Standard Orders (TSOs).

DecaBDE was likely also used in electronic parts for trains, ships, and elsewhere in the transportation industry for which there was not direct stakeholder representation in the partnership.

Box 2-4: DecaBDE is used in the following aviation and automotive applications

Aviation uses:

- Electrical wiring and cables
- Interior components
- Electric & electronic equipment
  - Navigation and telecommunications equipment
  - Computers and computer devices
  - Audio and video equipment
  - Electrical connectors
  - Galley appliances
  - Housings and internal components of entertainment units
  - Remote controls
  - Communications cables
  - Capacitor films
  - Cables
  - Circuit breakers
  - Cartridges and connectors
  - Air ducts for ventilation systems
  - Electrical ducts and fittings
  - Switches and connectors

Automotive uses:

- Electrical & electronic equipment
  - Battery cases
  - Battery trays
  - Engine controls
  - Electrical connectors
  - Components of radio, disk, GPS and computer systems
- Reinforced plastics
  - Instrument panels
  - Interior trim
- Under hood and internal parts
  - Terminal/fuse block
  - Higher amperage wire and cable jacketing (ignition wires)
- Fabric back coating
  - Rear deck
  - Upholstery
  - Sun visor
  - Head rest
  - Trim panel

Source: Bromine Science and Environmental Forum 2006; Baker 2011

2.2.5 Storage and Distribution Products

There are approximately three billion shipping pallets in use in the U.S., of which over 900 million are plastic (Pure Strategies Inc. prepared for the Maine Department of Environmental Protection 2010). According to the National Fire Protection Association (NFPA), plastic pallets that have not been treated with flame retardants are considered a greater fire hazard than wooden pallets. Plastic pallets are typically made of polyolefins, which are very combustible if they are not flame retarded.

Additionally, the International Fire Code (IFC), a widely adopted fire code but separate from the NFPA, requires plastic pallets be protected by an approved specialized engineered fire protection system unless they meet UL 2335 standards (see Table 2-2). Even though wood ignites at a lower temperature than plastic, once a fire begins, plastic burns at a higher temperature, and thus releases more heat (Pure Strategies Inc. for Maine Department of Environmental Protection 2010). NFPA 13 and IFC provide the basis for all state and local fire prevention laws and regulations governing warehouse construction and management throughout the country (Pure Strategies Inc. for Maine Department of Environmental Protection 2010).

To comply with fire standard NFPA 13, plastic pallets must comply with one of the two following options: (1) users must implement systems such as pallet storage management practices (e.g., how high the pallets are stacked and how close together stacks of pallets are) or sprinkler systems in warehouses that make it as safe as wooden pallets to use non-flame retarded plastic pallets, or (2) the pallets must pass tests consistent with ANSI/FM 4996 (see Table 2-2) that demonstrate that the fire hazard of the plastic pallet is less than or equal to the fire hazard of a wooden pallet (FM Approvals 2007). In order to meet the fire code specifications, flame retardants, often decaBDE, are integrated into plastic pallets to reduce the pallet's fire hazard (Levchik 2010; Pure Strategies Inc. for Maine Department of Environmental Protection 2010).

2.3 Flammability Tests

DecaBDE is used as a flame retardant in certain products either because of state or federal fire safety standards or for insurance purposes. Rather than specifying what flame retardants should be used, such standards specify the performance standards a product must meet under fire stress (Posner and Boras 2005). The stringency of the standard varies depending on the application (e.g., flammability requirements established for aircraft are much more stringent than those for clothing). Furthermore, decaBDE is sometimes added to products even without manufacturer requirements due to concerns for brand image and market pressure (Illinois Environmental Protection Agency 2007). Flammability standards may be developed by a variety of entities, including regulatory agencies such as the CPSC, or companies such as Underwriters Laboratory (UL).

Table 2-2 provides a brief overview of the flammability tests required for a variety of products in which decaBDE is used. This list is not comprehensive but does address many of the standards which lead to the use of decaBDE in the sectors discussed above.

Table 2-2: Summary of Flammability Tests Relevant to decaBDE Uses.

Test	Sectors and Products that Use Test	Description
UL 94	**Electrical and Electronic Equipment:** electronic enclosures	Assesses resistance to ignition from small internal (short circuit) or external (candle) ignition source. Small scale ignition resistance test.
UL 746 pt C	**Electrical and Electronic Equipment:** plastics in electronics and electrical parts	Based on UL 94.
NFPA 701	**Textiles:** public occupancy spaces: e.g., draperies of theatres, hotels, conference rooms, student dormitories	Assesses the propagation of a flame beyond the area exposed to the ignition source. A burner flame is applied for 45 seconds. To pass the test an average weight loss for ten specimens must be less than forty percent and fallen fragments should not burn more than two seconds.
California Technical Bulletin (TB)-133	**Textiles:** high risk occupancy areas: e.g., furniture of nursing homes, hospitals, prisons, hotels	Uses a full scale piece of furniture or mock up. Designed as a screening test. The fabric is exposed to a 1.5 inch methane flame for twelve seconds. Drips, burn time and char lengths are monitored along with temperature, mass lost, smoke and carbon monoxide.
Factory Mutual (FM) 4880	**Building and Construction:** public occupancy decorative wall and roof panels	Uses 750 lbs. of wood crib. The test ends when the flame reaches the structural limits or the crib stops burning. Tested material must not support self-propagating fire reaching structural limits.
American Society for Testing and Materials (ASTM) E-84	**Building and Construction:** insulation materials, foamed polyolefins, membranes, films sheets, ducting elements, ducts covering and insulation	Assesses the flame spread and smoke index. The tested material is mounted on the ceiling of the tunnel. Two gas burners are applied for ten minutes. The flame spread index and smoke index are calculated in relation to the flame spread and smoke density of red oak panels and concrete.
ASTM E648-10e1	**Building and Construction:** public occupancy floor tiles and carpeting	Measures the critical radiant flux, which is the minimum heat flux needed for materials to propagate the flame. The burning distance is converted to a critical radiant flux through the known flux distribution along the length of the test sample.
FMVSS 302	**Automotive and Aviation:** car seats, headliners, carpets, door panels, dash panels	Assesses flame spread from cigarettes and matches in the passenger compartment. A 1.5 inch flame is applied for fifteen seconds and flame travel and its speed on a horizontal specimen is recorded.
14 Code of Federal Regulations (CFR) Part 25 regulations: Sections 25.853, 25.855, 25.856, 25.869, Appendix F	**Aviation:** flooring, sidewalls, baggage compartment, insulation, ducting, interior parts, wiring	Materials and parts must successfully pass test(s) in order to show compliance. Nine 9 different tests are specified in the CFR and some materials/parts must pass multiple tests. Variations of configurations require individual testing. For specific details on the flammability tests see Appendix F of 14 CFR Part 25.

Test	Sectors and Products that Use Test	Description
UL 2335	**Shipping Pallets**	Assesses the performance of plastic pallets under fire stress. The goal of this test is to match the performance of plastic pallets to wood pallets. Six pallet stacks are ignited in the middle. The time to activate the first and last sprinkler, the number of sprinklers activated and the temperature at the ceiling are all recorded. Sprinklers are mounted above the stacks and are activated at 165°F. To pass the test no more than six sprinklers can be activated.
FM 4996	**Shipping Pallets**	This standard sets fire performance requirements for plastic pallets so that they can be assigned a classification as equivalent to wood pallets in an effort to determine the demand on a sprinkler system in the event of a fire. The test consists of sixteen stacks of pallets placed in a specified arrangement. Ignition is provided by four ignitors placed at the center of the array. The number of sprinklers that operate, the maximum ceiling temperature (gas and steel) at one and five minutes, the extent of the fire damage and the extent of the melted plastic pooling is recorded. These values are than compared to values for idle wood pallets. If the pallets tested meet or exceed the performance criteria limits it is designated "equivalent to wood."

Sources: FM Approvals 2007; Levchik 2010; Baker 2011

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3 Background on Flame Retardants

This chapter begins with background information on flame retardants, including their classification (Section 3.1). Section 3.2 presents the flame retardants included in this assessment and Section 3.3 discusses those which were considered but excluded from the assessment. Section 3.4 presents the mechanisms by which flame retardants reduce or prevent combustion.

3.1 General Information on Flame Retardants

Flame retardants decrease the ignitability of materials and inhibit the combustion process, limiting the amount of heat released. The simplest way, in theory, of preventing polymer combustion is to design the polymer so that it is thermally stable. Thermally stable polymers are less likely to decompose into combustible gases under heat stress, which prevents combustion from initiating. Because thermally stable polymers are often difficult and expensive to process and may have performance limitations, manufacturers use other means, such as flame-retardant chemicals, to impart flame-retardant properties to polymers.

Flame retardants decrease the likelihood of a fire occurring and/or decrease a range of undesirable consequences of a fire (Lyons 1970; Cullis and Hirschler 1981). However, in other instances the incomplete combustion resulting from the use of flame retardants, where oxidation and/or thermal transfer are inhibited, can produce negative by-products (e.g., carbon monoxide). These by-products are in addition to the production of other toxic chemicals (e.g., halogenated dioxins and furans) created by the combustion of materials containing flame retardants.

Fire occurs in three stages: (1) thermal decomposition, where the solid, or condensed phase, breaks down into gaseous decomposition products as a result of heat; (2) combustion chain reactions in the gas phase, where thermal decomposition products react with an oxidant (usually air) and generate more combustion products, which can then propagate the fire and release heat; and (3) transfer of the heat generated from the combustion process back to the condensed phase to continue the thermal decomposition process (Hirschler 1992; Beyler and Hirschler 2002).

The basic mechanisms of flame retardancy will vary depending on the flame retardant and polymer system. Flame retardants can be classified based on the phase (solid or gas) in which they act to reduce or prevent propagation of flame. Other flame retardants may form protective barriers over a polymer which may insulate the flammable polymer from heat or reduce the amount of polymer that is available to burn as fuel. In either state, gaseous or condensed, flame retardants will act to decrease the release rate of heat (Hirschler 1994), thus reducing the burning rate, flame spread, and/or smoke generation (Morose 2006). These mechanisms are discussed further in Section 3.4.

Typically, flame retardants contain one or more of the following elements: chlorine, bromine, aluminum, boron, nitrogen, phosphorus, or silicon (Lyons 1970; Cullis and Hirschler 1981). There are a number of alternatives and synergists that are also effective. Some elements, such as zinc (often used as zinc borate or zinc stannate) and molybdenum (often used as ammonium molybdates), are effective primarily as smoke suppressants in mixtures of flame retardants. In addition, antimony trioxide can serve as an effective synergist in combination with halogenated flame retardants.

The amount of flame retardant needed to pass a given flammability standard varies due to a number of factors. In general, the lowest levels of flame retardants are required with bromine-based chemistries, and higher levels are required when using mineral-type compounds. Ranges of typical "loading levels" (how much of a flame retardant is added to a material) for common flame retardants are shown in Table 3-1. Loading levels also depend on the polymers in which the flame retardant is used. For example, bromine-based flame retardants are used in a wide variety of products (e.g., polyolefins, styrene, polyamides (PAs), polyesters, polycarbonates (PCs) and textiles) and thus have a wide range of loading levels[8]. This is demonstrated by the fact that when used in polyesters, bromine-based flame retardants have a loading level of about 8 percent, whereas when bromine-based flame retardants are used in textiles, they are usually at about a 17 percent loading. On the other hand, the flame retardants that are not used in such a wide variety of products have much smaller loading ranges. For example, chlorophosphates have a 9 percent loading in epoxy resins and a 10 percent loading in polyurethane and are not reportedly used with other polymers (Weil and Levchik 2009).

Table 3-1: Typical Loading Levels[8] of Common Flame Retardants

Type of Flame Retardant	Loading (wt %)
Bromine-based	2 to 25%[1]
Aluminum Hydroxide	13 to 60%
Magnesium Hydroxide	53 to 60%
Chlorophosphates	9 to 10%
Organophosphorus	5 to 30%

[1] Polyethylene (PE) can require up to 31% of a bromine based flame retardant and 7-8 % antimony trioxide. However, this is rarely practiced in the market thus the upper limit displayed above is 25%.
Source: Weil and Levchik 2009

Flame-Retardant Classification

Flame retardants can be classified into four main categories according to chemical composition:

- *Inorganic*: This category includes flame retardants and synergists such as silicon dioxide, metal hydroxides (e.g., aluminum hydroxide and magnesium hydroxide), antimony compounds (e.g., antimony trioxide), boron compounds (e.g., zinc borate – which is often used as a synergist for both halogenated and non-halogenated flame retardants), and other metal compounds (molybdenum trioxide). As a group, these flame retardants represent the largest fraction of total flame retardants in use (Norwegian Pollution Control Agency 2009).

- *Halogenated*: These flame retardants are primarily based on bromine and chlorine. Typical halogenated flame retardants are halogenated paraffins, halogenated aliphatic and aromatic compounds, and halogenated polymeric materials. Some halogenated flame retardants also contain other elements, such as phosphorus or nitrogen. The effectiveness

[8] These loading levels can be measured in percent by weight (i.e., percent in relation to the total weight of the components or final product) or in parts per hundred part of resin (phr) (i.e., all phrs will be over 100). Information in Table 3-1 is presented as a percentage of the weight of the final product.

of halogenated additives, as discussed below in Section 3.4, is due to their interference with volatile substances which are created in the combustion process, decreasing their combustibility. Brominated compounds represent approximately 18 to 21 percent (by volume) of the global flame-retardant production (BCC Research 2006; Cusack 2007).

- *Phosphorus-based*: This category represents about 20 percent (by volume) of the global production of flame retardants and includes organic and inorganic phosphates, phosphonates, and phosphinates as well as red phosphorus, covering a wide range of phosphorus compounds with different oxidation states. There are also halogenated phosphate esters, often used as flame retardants for polyurethane foams or as flame-retardant plasticizers, but not commonly used in electronics applications (Hirschler 1998; Green 2000; Weil and Levchik 2004).

- *Nitrogen-based*: These flame retardants include melamine and melamine derivatives (e.g., melamine cyanurate, melamine polyphosphate). Nitrogen-containing flame retardants are often used in combination with phosphorus-based flame retardants, with both elements in the same molecule (Morose 2006).

Halogenated flame retardants are commonly blended with a synergist, such as antimony trioxide. A synergist multiplicatively enhances the flame retardant effect. Many flame-retardant synergists do not have significant flame-retardant properties by themselves; their addition increases the overall effectiveness of the flame-retardant system. It should also be noted that the synergists may be very system specific; they are not universal. For example, antimony trioxide only shows flame retardant synergism with halogenated flame retardants and has no effect when combined with inorganic, phosphorus, or nitrogen-based flame retardants.

Flame retardants also can be classified by how they are incorporated into a polymer – additively or reactively. No reactive-type flame retardants were identified as alternatives to decabromodiphenyl ether (decaBDE) in this assessment.

- *Additive:* Additive flame retardants are incorporated into polymers via physical mixing, and are not chemically bound to the polymer. Flame-retardant compounds are mixed with existing polymers without undergoing any chemical reactions. As a result, the polymer/additive mixture is less susceptible to combustion than the polymer alone. Since additive flame retardants can be incorporated into the product up until the final stages of manufacturing, it is usually easier for manufacturers to use additive flame retardants than reactive flame retardants.

- *Reactive:* Reactive flame retardants are incorporated into polymers via chemical reactions and must be incorporated at an early stage of manufacturing. Once introduced, they become a permanent part of the polymer structure – i.e., the chemically-bound reactive flame-retardant chemicals cease to exist as separate chemical entities. As a result, reactive flame retardants have a greater effect on the chemical and physical properties of the polymer into which they are incorporated than do additive flame retardants. For examples of reactive flame retardants, refer to the Flame Retardants in Printed Circuit Boards Draft Report (U.S. EPA 2008c).

Flame retardants can also be coated on the external surface of the polymer to form a protective barrier or to improve their compatibility with the polymeric matrix.

Both reactive and additive flame retardants can significantly change the properties of the polymers into which they are incorporated. Each flame retardant polymer combination is unique. For example, they may change the viscosity, flexibility, density, electrical properties, tensile strength, and flexural strength; and may also increase the susceptibility of the polymers to photochemical and thermal degradation.

3.2 Flame Retardants Included in this Assessment

With the assistance of the partnership, the U.S. Environmental Protection Agency (EPA) identified 32 alternatives to decaBDE which fit the scope of this project: to identify potentially functional, viable alternatives for use in the identified polyolefins, styrenics, engineering thermoplastics, thermosets, elastomers or waterborne emulsions and coatings (see Chapter 1). It is important to stress that these alternatives were not chosen based on environmental preferability but based on their functionality and viability. These alternatives were identified through the following process:

1) EPA developed an initial list of alternatives based on a review of the literature (Posner and Boras 2005; Danish Ministry of the Environment 2007; European Chemicals Bureau 2007; Washington State Department of Health 2008; Pure Strategies Inc. prepared for the Maine Department of Environmental Protection 2010) and consultation with industry experts.

2) This list was presented to the partnership, and through multiple discussions EPA confirmed which chemicals were viable alternatives and identified any additional alternatives which were not found through the literature review process.

3) Chemicals that were initially included as potential alternatives (identified through the literature review) but were not deemed viable by the experts on the partnership were excluded from the assessment (see Section 3.3).

Table 3-2 presents the viable flame retardant alternatives included in this assessment, along with a summary of the polymers in which they are most often used, and end-use products into which the polymers are incorporated. The chemicals in Table 3-2 are additive flame retardants unless otherwise noted. Their modes of flame-retardant action are also given in Table 3-2 and discussed in Section 3.4. These modes of action include:

- CA - C: Chemical action in condensed phase,
- CA - G: Chemical action in gas phase,
- HS: Heat sink,
- CF: Char former,

- I: Intumescent[9], and
- D: Dilution effect.

[9] Intumescence is when a compound swells as a result of heat exposure, thus increasing in volume, and decreasing in density.

Table 3-2: Summary of Chemicals for Assessment with Polymer and End-Use Application

Flame Retardant Chemicals for Assessment	Chemical Abstracts Service Registry Number (CASRN)	Polymer Applications[1]	End-Use Applications[2]									Mode of Action[3]
			Electronics	Wire and Cable	Public Buildings	Construction Materials	Automotive	Aviation	Storage and Distribution Products	Textiles	Waterborne emulsions & coatings	
Decabromodiphenyl ether, decaBDE	1163-19-5	Chlorinated polyethylene (CPE)	✓	✓								CA - G + CA - C (with metal hydroxide [HS])
		Elastomers	✓	✓	✓	✓	✓	✓				
		Emulsions								✓	✓	
		Engineering Thermoplastic	✓				✓				✓	
		High-impact polystyrene (HIPS)	✓									
		Polyethylene (PE)	✓	✓	✓	✓	✓	✓	✓			
		Polypropylene (PP)	✓	✓			✓		✓			
		Thermosets	✓		✓	✓						
Aluminum diethylphosphinate	225789-38-8	Elastomers	✓	✓			✓	✓				CF + I +HS
		Epoxy resins	✓				✓	✓				
		Polyamide (PA)	✓				✓	✓		✓		
		Polybutylene terephthalate (PBT)	✓				✓	✓				
		Polyethylene terephthalate (PET)	✓				✓	✓		✓		
		Thermoplastic polyurethane (TPU)		✓								

[1]If a polymer is not listed for any specific flame retardant, then the flame retardant is not functional in that material application
[2]All categories may include military uses
[3]CA - C: Chemical action in condensed phase, CA - G: Chemical action in gas phase. Physical action can be HS (Heat sink), CF (Char former), I (Intumescent), or D (Dilution effect)

Flame Retardant Chemicals for Assessment	Chemical Abstracts Service Registry Number (CASRN)	Polymer Applications[1]	End-Use Applications[2]									Mode of Action[3]
			Electronics	Wire and Cable	Public Buildings	Construction Materials	Automotive	Aviation	Storage and Distribution Products	Textiles	Waterborne emulsions & coatings	
Aluminum hydroxide	21645-51-2; 8064-00-4	Elastomers		✓	✓	✓	✓	✓				HS + I
		Emulsions								✓		
		Ethylene vinyl acetate (EVA)		✓	✓	✓	✓	✓				
		PE		✓	✓	✓	✓	✓				
		Thermosets	✓		✓	✓	✓	✓			✓	
Ammonium polyphosphate, APP	68333-79-9; 14728-39-3	Elastomers		✓								CA - C + I
		Emulsions								✓	✓	
		PE		✓	✓	✓			✓			
		PP	✓	✓	✓	✓	✓		✓			
		Thermosets			✓	✓		✓	✓			
Antimony trioxide, antimony oxide (Used as a synergist only)	1309-64-4	Elastomers	✓	✓	✓	✓	✓	✓	✓		✓	CA - G (synergists)
		Emulsions							✓		✓	
		Engineering Thermoplastic	✓	✓	✓	✓	✓	✓				
		HIPS	✓	✓	✓	✓	✓	✓	✓			
		PE	✓	✓	✓	✓	✓	✓	✓			
		PP	✓	✓	✓	✓	✓	✓	✓			
		Polyvinyl chloride (PVC)	✓	✓	✓	✓	✓			✓		
		Thermosets	✓		✓	✓						

[1]If a polymer is not listed for any specific flame retardant, then the flame retardant is not functional in that material application
[2]All categories may include military
[3]CA - C: Chemical action in condensed phase, CA - G: Chemical action in gas phase. Physical action can be HS (Heat sink), CF (Char former), I (Intumescent), or D (Dilution effect)

Flame Retardant Chemicals for Assessment	Chemical Abstracts Service Registry Number (CASRN)	Polymer Applications[1]	End-Use Applications[2]									Mode of Action[3]
			Electronics	Wire and Cable	Public Buildings	Construction Materials	Automotive	Aviation	Storage and Distribution Products	Textiles	Waterborne emulsions & coatings	
Bis (hexachlorocyclopentadieno) cyclooctane	13560-89-9	CPE	✓	✓							✓	CA - G + CF; CA - G + CA - C (with metal hydroxide oxide [HS])
		Elastomers	✓	✓	✓	✓						
		Engineering Thermoplastic	✓									
		HIPS	✓									
		PE	✓	✓	✓	✓						
		PP	✓	✓								
		Thermosets	✓		✓	✓					✓	
Bisphenol A bis-(diphenyl phosphate) (reaction products), BAPP, BDP or DPADP	5945-33-5; 181028-79-5 (reaction products)	Polyphenylene ether – high-impact polystyrene (PPE-HIPS)	✓									CA - C + CF; (synergist)
		Polycarbonate (PC)	✓									
		Polycarbonate-acrylonitrile butadiene styrene (PC-ABS)	✓									

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[2]All categories may include military
[3]CA - C: Chemical action in condensed phase, CA - G: Chemical action in gas phase. Physical action can be HS (Heat sink), CF (Char former), I (Intumescent), or D (Dilution effect)

Flame Retardant Chemicals for Assessment	Chemical Abstracts Service Registry Number (CASRN)	Polymer Applications[1]	End-Use Applications[2]									Mode of Action[3]
			Electronics	Wire and Cable	Public Buildings	Construction Materials	Automotive	Aviation	Storage and Distribution Products	Textiles	Waterborne emulsions & coatings	
Brominated epoxy resin end-capped with tribromophenol	135229-48-0	Acrylonitrile butadiene styrene (ABS)	✓									CA - G + CA - C (with metal hydroxide [HS])
		HIPS	✓									
		Nylon	✓				✓					
		PBT	✓				✓					
		Unsaturated polyesters (UPE)			✓	✓						
Brominated polyacrylate	59447-57-3	PA	✓				✓					CA - G
		PBT	✓				✓					
		PP	✓				✓		✓			
		PE							✓			
Brominated polystyrene	88497-56-7	PA	✓				✓					CA - G
		PET	✓									
		PBT	✓									
		Thermoplastic polyester	✓									
		Thermoset polyester	✓									

[1]If a polymer is not listed for any specific flame retardant, then the flame retardant is not functional in that material application
[2]All categories may include military
[3]CA - C: Chemical action in condensed phase, CA - G: Chemical action in gas phase. Physical action can be HS (Heat sink), CF (Char former), I (Intumescent), or D (Dilution effect)

Flame Retardant Chemicals for Assessment	Chemical Abstracts Service Registry Number (CASRN)	Polymer Applications[1]	End-Use Applications[2]									Mode of Action[3]
			Electronics	Wire and Cable	Public Buildings	Construction Materials	Automotive	Aviation	Storage and Distribution Products	Textiles	Waterborne emulsions & coatings	
Confidential brominated epoxy polymer #1, Confidential brominated epoxy polymer #2, Confidential brominated epoxy polymer mixture #1, Confidential brominated epoxy polymer mixture #2	Confidential	ABS	✓									CA - G
		HIPS	✓									
		PE							✓			
Confidential brominated polymer	Confidential	CPE	✓	✓							✓	CA - G
		Elastomers	✓	✓	✓	✓	✓		✓			
		Emulsions								✓	✓	
		Engineering Thermoplastics	✓	✓			✓				✓	
		HIPS	✓									
		PE	✓	✓	✓	✓	✓		✓			
		PP	✓	✓			✓		✓		✓	
		Thermosets	✓		✓	✓						
Decabromodiphenyl ethane, Ethane 1, 2 – (bispentabromophenyl), EBP, DBDPE	84852-53-9	CPE	✓	✓							✓	CA - G + CA - C (with metal hydroxide [HS])
		Elastomers	✓	✓	✓	✓	✓		✓			
		Emulsions								✓	✓	
		Engineering Thermoplastics	✓	✓			✓				✓	
		HIPS	✓									
		PE	✓	✓	✓	✓	✓		✓			
		PP	✓	✓			✓		✓		✓	
		Thermosets	✓		✓	✓						

[1]If a polymer is not listed for any specific flame retardant, then the flame retardant is not functional in that material application
[2]All categories may include military
[3]CA - C: Chemical action in condensed phase, CA - G: Chemical action in gas phase. Physical action can be HS (Heat sink), CF (Char former), I (Intumescent), or D (Dilution effect)

Flame Retardant Chemicals for Assessment	Chemical Abstracts Service Registry Number (CASRN)	Polymer Applications[1]	End-Use Applications[2]									Mode of Action[3]
			Electronics	Wire and Cable	Public Buildings	Construction Materials	Automotive	Aviation	Storage and Distribution Products	Textiles	Waterborne emulsions & coatings	
Ethylene bis-tetrabromophthalimide, EBTBP	32588-76-4	CPE		✓							✓	CA - G; CA - C (Increased thermal stability)
		Elastomers				✓						
		Engineering Thermoplastic	✓									
		HIPS	✓									
		PE	✓	✓	✓	✓	✓		✓			
		PP	✓	✓	✓	✓	✓		✓			
Magnesium hydroxide[4]	1309-42-8	Elastomers		✓	✓	✓	✓	✓				CF + HS
		EVA		✓	✓	✓	✓	✓				
		PA	✓									
		PE		✓	✓	✓	✓	✓	✓			
		PP		✓	✓	✓	✓	✓	✓		✓	
Melamine cyanurate	37640-57-6	PA	✓		✓	✓	✓	✓		✓	✓	HS + D
		PBT	✓		✓	✓	✓	✓		✓	✓	
		TPU	✓		✓	✓	✓	✓		✓	✓	
		UPE	✓		✓	✓	✓	✓		✓	✓	

[1]If a polymer is not listed for any specific flame retardant, then the flame retardant is not functional in that material application
[2]All categories may include military
[3]CA - C: Chemical action in condensed phase, CA - G: Chemical action in gas phase. Physical action can be HS (Heat sink), CF (Char former), I (Intumescent), or D (Dilution effect)
[4] Previously assessed by Design for the Environment (DfE) in other alternatives assessments (http://www.epa.gov/dfe/alternative_assessments.html)

Flame Retardant Chemicals for Assessment	Chemical Abstracts Service Registry Number (CASRN)	Polymer Applications[1]	End-Use Applications[2]									Mode of Action[3]
			Electronics	Wire and Cable	Public Buildings	Construction Materials	Automotive	Aviation	Storage and Distribution Products	Textiles	Waterborne emulsions & coatings	
Melamine polyphosphate[4]	218768-84-4	Epoxy resins	✓		✓	✓	✓	✓			✓	HS + D + CF
		PA	✓		✓	✓	✓	✓			✓	
		PBT	✓		✓	✓	✓	✓			✓	
		PE							✓			
		Phenolic based composites	✓		✓	✓	✓	✓			✓	
		PP							✓			
		TPU	✓		✓	✓	✓	✓			✓	
		UPE	✓		✓	✓	✓	✓			✓	
N-alkoxy hindered amine reaction products	191680-81-6	PE thin films				✓				✓		CA - G
		PP thin films and fibers				✓				✓		
Phosphonate oligomer[5]	68664-06-2	Thermosets	✓		✓	✓						CA - C; CF
Polyphosphonate	68664-06-2	Elastomers	✓	✓	✓	✓	✓	✓				CA - C; CF
		Engineering Thermoplastic	✓		✓	✓	✓	✓		✓		
Poly[phosphonate-co-carbonate]	77226-90-5	Elastomers	✓	✓	✓	✓	✓	✓				CA - C; CF
		Engineering Thermoplastic	✓		✓	✓	✓	✓				

[1]If a polymer is not listed for any specific flame retardant, then the flame retardant is not functional in that material application
[2]All categories may include military
[3]CA - C: Chemical action in condensed phase, CA - G: Chemical action in gas phase. Physical action can be HS (Heat sink), CF (Char former), I (Intumescent), or D (Dilution effect)
[4]Previously assessed by Design for the Environment (DfE) in other alternatives assessments (http://www.epa.gov/dfe/alternative_assessments.html)
[5]Also available as a reactive oligomer to react with the host polymer system

Flame Retardant Chemicals for Assessment	Chemical Abstracts Service Registry Number (CASRN)	Polymer Applications[1]	End-Use Applications[2]									Mode of Action[3]
			Electronics	Wire and Cable	Public Buildings	Construction Materials	Automotive	Aviation	Storage and Distribution Products	Textiles	Waterborne emulsions & coatings	
Red Phosphorus	7723-14-0	Elastomers		✓								CA - G + CA - C
		Emulsions					✓				✓	
		Epoxy resins	✓				✓	✓			✓	
		PA	✓	✓				✓				
		PA 66 GF	✓									
		PP	✓	✓								
Resorcinol bis-diphenylphosphate, RDP	125997-21-9; 57583-54-7	PPE-HIPS	✓									CA - C + CF; synergist
		PC-ABS	✓									
Substituted amine phosphate mixture	66034-17-1 and confidential	Elastomers	✓	✓	✓	✓	✓	✓	✓			CA - C; CF + I
		EVA		✓	✓	✓	✓	✓				
		PE	✓	✓	✓	✓	✓	✓	✓			
		PP	✓	✓	✓	✓	✓	✓	✓			
		TPU	✓	✓	✓	✓	✓	✓				
Tetrabromobisphenol A bis (2,3-dibromopropyl ether)	21850-44-2	Elastomers	✓		✓	✓	✓					CA - G + CA - C (with metal hydroxide [HS])
		PP	✓		✓	✓	✓					
TBBPA glycidyl ether & TBBPA polymers	68928-70-1	ABS	✓									CA - G + CA - C (with metal hydroxide [HS])
		HIPS	✓									
		Nylon	✓				✓					
		PBT	✓				✓					
		UPE			✓	✓						

[1]If a polymer is not listed for any specific flame retardant, then the flame retardant is not functional in that material application
[2]All categories may include military
[3]CA - C: Chemical action in condensed phase, CA - G: Chemical action in gas phase. Physical action can be HS (Heat sink), CF (Char former), I (Intumescent), or D (Dilution effect)

Flame Retardant Chemicals for Assessment	Chemical Abstracts Service Registry Number (CASRN)	Polymer Applications[1]	End-Use Applications[2]									Mode of Action[3]
			Electronics	Wire and Cable	Public Buildings	Construction Materials	Automotive	Aviation	Storage and Distribution Products	Textiles	Waterborne emulsions & coatings	
Triphenyl phosphate (TPP)[4]	115-86-6	PPE-HIPS	✓									CA - C + CF
		PC-ABS	✓									
Tris(tribromoneopentyl) phosphate	19186-97-1	PP	✓		✓	✓				✓		CA - G + CA - C + CF + I
Tris(tribromophenoxy) triazine, Tris(tribromophenyl) cyanurate	25713-60-4	ABS	✓									CA - G + CF + D
		HIPS	✓									
Zinc borate (Synergist for halogen and Non-halogen)	138265-88-0; 1332-07-6	EVA	✓	✓	✓	✓	✓	✓			✓	HS + CF + CA - C
		PE	✓	✓	✓	✓	✓	✓	✓			
		PP	✓	✓	✓	✓	✓	✓	✓			

[1]If a polymer is not listed for any specific flame retardant, then the flame retardant is not functional in that material application
[2]All categories may include military
[3]CA - C: Chemical action in condensed phase, CA - G: Chemical action in gas phase. Physical action can be HS (Heat sink), CF (Char former), I (Intumescent), or D (Dilution effect)
[4]Previously assessed by DfE in other alternatives assessments (http://www.epa.gov/dfe/alternative_assessments.html)
Source: Personal communication with members of the partnership.

3.3 Flame Retardants Not Included in this Assessment

In addition to the chemicals listed in Table 3-2, the partnership considered other flame retardants for the assessment, including individual chemicals and materials. Section 3.3.1 describes chemicals that were identified as possible alternatives to decaBDE and the reasons they were excluded from the assessment. Sections 3.3.2 and 3.3.3 describe two general types of nanomaterials that were not assessed because EPA does not have sufficient experience to apply data from one form of a chemical substance (such as a bulk material) to a particular nanoform of that chemical.

3.3.1 Chemicals That Were Excluded from this Assessment

The chemicals listed in this section were identified as possible alternatives to decaBDE, but were not included in the alternatives assessment. Reasons for exclusion included:

- Not commercially available[10];
- The flame retardant is a blend of which a majority of the chemicals are included in the assessment;
- Compared to other chemicals being assessed, the flame retardant is used or has the potential to be used in only small quantities;
- Outside the scope of the project: not a flame retardant or not relevant to materials in the scope;
- The Hazard Evaluation Criteria (U.S. EPA 2011b) cannot yet be applied to evaluation of nanomaterials;
- Regulatory action has been proposed or implemented making future use unlikely;
- Will be addressed qualitatively in this report;
- Limited use as a decaBDE replacement due to toxic byproducts or regulations; and
- Not functional in materials in which decaBDE has been used.

A summary of the chemicals which were discussed but not included in this assessment are listed in Table 3-3 with the reason for exclusion. Additionally, it is likely that the Partnership omitted some potential alternatives. For example, TBBPA carbonate oligomer (CASRN 94334-64-2; 71342-77-3) was mentioned but not identified as a high priority alternative and tetradecabromo-1,4-diphenoxybenzene (CASRN 58965-66-5) was not brought up during the survey of available alternatives. These chemicals and others not yet identified or currently under development may be included in future versions of this report.

[10] Some flame retardants that are currently in the process of market commercialization are included in the list of flame retardants in Section 3.2.

Table 3-3: Chemicals Considered but Not Included in the Final Alternatives Assessment

Chemical Name	CASRN	Justification for Exclusion
1,2 - bis(pentabromophenoxy) ethane	61262-53-1	This chemical is no longer on the market. Neither is the similar but lower brominated 1,2 - bis(tribromophenoxy) ethane.
Ammonium polyphosphate + melamine + pentaerythritol		The flame retardant is a blend, of which a majority of the chemicals are included in the assessment.
Boehmite (Aluminum hydroxide oxide)	1318-23-6	Compared to other chemicals being assessed, it is used and/or has the potential to be only in small quantities. A similar but different compound to aluminum hydroxide.
Calcium molybdate (Powellite)	7789–82–4	This is more of a smoke suppressant than a stand-alone flame retardant and is for PVC.
Diphenyl cresyl phosphate (DPK)	26444-49-5	DPK is mostly used as plasticizer in PVC, and is not used as a decaBDE replacement.
Ethylenediamine-o-phosphate	14852-17-6	Compared to other chemicals being assessed, it is used and/or has the potential to be used in small quantities.
Green Armor	Unknown	The chemical has not yet completed the Premanufacture Notice (PMN) process at EPA.[1] The manufacturer prefers not to include this substance in the DfE process until PMN review is complete.
Huntite / hydromagnesite $Mg_3Ca(CO_3)(OH)_23H_2O$		Compared to other chemicals being assessed, it is used and/or has the potential to be used in small quantities.
KSS - Potassium 3-(phenylsulfonyl)benzenesulfonate	63316-43-8 (monosulfonate); 63316-33-6 (disulfonate)	KSS is mainly used in PCs, and not in PC blends.
Mesoporous silicate particles (MSPs)		The DfE Hazard Evaluation Criteria (U.S. EPA 2011b) cannot yet be applied to evaluation of nanomaterials. EPA does not have sufficient experience to apply data from one form of a chemical substance (such as a bulk material) to a particular nanoform of that chemical. These materials are not assessed in this report but they are still of interest and are discussed in Section 3.3.3.

[1] Anyone who plans to manufacture or import a new chemical substance for a non-exempt commercial purpose is required by section 5 of the Toxic Substances Control Act (TSCA) to provide EPA with a PMN which must be submitted at least 90 days prior to the manufacture or import of the chemical.

Chemical Name	CASRN	Justification for Exclusion
Nanoclays		The DfE Hazard Evaluation Criteria (U.S. EPA 2011b) cannot yet be applied to evaluation of nanomaterials. EPA does not have sufficient experience to apply data from one form of a chemical substance (such as a bulk material) to a particular nanoform of that chemical. These materials are not assessed in this report but they are still of interest and are discussed in Section 3.3.3.
Pentaerythritol	115-77-5	In contrast to melamine cyanurate and melamine polyphosphate, which are included in the assessment and can be used as flame retardants by themselves, pentaerythritol must be combined with melamine AND a phosphate to be effective and so is not included in this assessment as a stand-alone flame retardant
Phosphonic acid, (3-{[hydroxymethyl]amino}-3-oxopropyl)-dimethyl ester	20120–33–6	Limited use as a decaBDE replacement: this compound's use in the United States is almost zero because it is used with compounds which can release formaldehyde.
Poly(aryl ether ketone) (PAEK – various suppliers – covers PEK, PEEK, PEKK, etc.)		Will be addressed qualitatively in the report: this is an inherently flame retardant (IFR) polymer (see Section 3.3.2).
Polyetherimde	61128-46-9	Will be addressed qualitatively in the report: this is an IFR polymer (see Section 3.3.2)
PET with built-in phosphorus on polyester backbone	25038-59-9	Not effective in most materials where decaBDE is currently used to meet required flammability standards. Therefore, the use of this chemical is limited and not a priority for assessment.
Short and Medium Chain Chloroparaffins	63449-39-8; 85535-85-9	Regulatory action has been proposed or implemented for short chain chloroparaffins – the chemical will not be on the market in the future. Medium and long chained chloroparaffins are being further evaluated to determine whether their manufacturing, processing, distribution in commerce, and/or use should also be addressed (U.S. EPA 2009b).
Tetrabromobisphenol A	79-94-7	Was not identified as a prevalent alternative to decaBDE. Additionally, a full discussion of TBBPA manufacturing, process and hazard is provided in a previous DfE report (U.S. EPA 2008c).
Tetrakis (hydroxymethyl) phosphonium, urea, chloride salts	124–64–1	Not effective in most materials where decaBDE is currently used to meet required flammability standards. Therefore, the use of this chemical is limited and not a priority for assessment.
Tricresyl phosphate	1330–78–5	Outside of the scope of this project: this is a plasticizer for PVC.

Chemical Name	CASRN	Justification for Exclusion
Tris (1,3-dichloropropyl-2) phosphate	13674–87–8	Previously assessed and limited use as a decaBDE replacement: this chemical is not used as a primary flame retardant in textile backcoatings and TDCPP was reviewed in DfE's Furniture Flame Retardancy Report (U.S. EPA 2005a).
Tris (2-hydroxyethyl) isocyanurate	839-90-7	Not a flame retardant; part of a curing system for coatings.
Zinc molybdate	13767–32–3	Limited use as a decaBDE replacement: this is a potential alternative synergist to antimony trioxide when used in textiles. It is also a smoke suppressant. However, it is not a particularly viable alternative synergist because of cost and municipal water discharge restrictions.

3.3.2 Inherently Flame Retardant Materials

IFR materials meet fire code standards without special processing or chemical additives. IFRs are not flammable, which means that the protection is built into the fiber and is less likely to be worn away or washed out (DuPont 2010). IFRs can be used in a multitude of materials, and are not limited to fibers. IFR technologies are used in textiles, electronics, aircraft, and ground transportation vehicles and may be used in place of decaBDE in some instances. Table 3-4 includes a few examples of IFRs, their attributes, and end-use products relevant to this assessment. This report assessed flame retardant additives, and did not assess polymers in which these additives are used, nor these IFR materials, for their own inherent hazard.

Table 3-4: Examples and Descriptions of Inherently Flame Retardant Materials

Inherently Flame Retardant Material	Description and Attributes	End Uses Relevant to this Assessment
Graphite impregnated foam	▪ Relatively new technology which is self-extinguishing and highly resistant to combustion. ▪ Can meet airline fire safety standards for the seats with a reduced dependency on flame-retarded fabric. (U.S. EPA 2005a)	▪ Largely used in niche markets, e.g., general aircraft seating (U.S. EPA 2005a)
Low heat release plastics (Nomex, Teflon)	▪ Characterized by lower heat release capacities. ▪ High melt temperature (if any), hard to process using conventional plastics processing methods. (Walters and Lyon 2003)	▪ Aircraft ▪ Firefighter apparel ▪ Soldier protection fabric ▪ Flame retardant tents (Nagarajan 2012)
Polyimides (PI)	▪ Linear polymers which contain a ring structure along the backbone. This backbone structure gives the polymer good high temperature properties. ▪ PIs have excellent physical properties and are used in applications where parts are exposed to harsh environments. ▪ Oxidative stability allows them to withstand continuous service in air at temps of 260^0C. PIs will burn but they have a self-extinguishing property. (Modern Plastics and Charles A. Harper 1999)	▪ Wire enamel ▪ Bearings for appliances in aircrafts, seals and gaskets ▪ Flexible wiring and electrical motor insulation – used with film version of PI (Modern Plastics and Charles A. Harper 1999)
Polyketones	▪ Family of aromatic polyether ketones includes structures which vary in the location and number of ketonic and ether linkages on their repeat units including PEK, PEEK, PEEKK and other combinations. ▪ All have very high thermal properties due to their aromaticity of their back bones and are readily processed via injection molding. ▪ Toughness is high for such high-heat resistance materials. ▪ Low moisture absorption and good hydrolytic stability lend these materials to their applications. (Modern Plastics and Charles A. Harper 1999)	▪ Airplane and automobile engines (Modern Plastics and Charles A. Harper 1999)

Inherently Flame Retardant Material	Description and Attributes	End Uses Relevant to this Assessment
Geopolymers	▪ Polysialate family of inorganic matrices. ▪ Geopolymer is a two-part system consisting of an alumina liquid and a silica powder that cures at around 150°C. ▪ Low curing temperatures, high temperature resistance, and low cost. ▪ Compatible with carbon, glass, Kevlar, steel, cellulosics. (Nagarajan 2012)	▪ Items with high-use temperatures anticipated ▪ Engine exhaust system ▪ Aircrafts (Nagarajan 2012)
Liquid Crystal Polymer (LCP)	▪ Aromatic copolyesters - the presence of phenyl rings in the backbone gives chain rigidity, forming rod-like chain structures. ▪ Self-reinforcing with high mechanical properties. ▪ Known for high-temperature resistance, particularly heat-distortion temperature. ▪ Excellent mechanical properties, especially in flow direction. Good electrical insulation properties and low flammability. LCPs show little dimensional change when exposed to high temperatures and a low coefficient of thermal expansion. ▪ Can be high priced and often exhibit poor abrasion resistance. ▪ Can be injection molded on conventional equipment and regrind may be used. (Modern Plastics and Charles A. Harper 1999)	▪ Automotive ▪ Electrical chemical processing ▪ Household applications such as in ovens or microwave cookware (Modern Plastics and Charles A. Harper 1999)
Polyarylates	▪ Amorphous, aromatic polyesters prepared from dicarboxylic acids and bisphenols. ▪ Aromatic rings give the polymer good temperature resistance. ▪ Shows good toughness and ultraviolet resistance. ▪ Transparent and has good electrical properties. ▪ Abrasion resistance of polyarylates is superior to PC. ▪ Extreme rigidity of polymer chains (due to aromatic rings) leads to difficulty in processing. ▪ Polyarylates, while having low heat release, may not be IFR in all fire risk scenarios. (Modern Plastics and Charles A. Harper 1999)	▪ Automotive applications such as door handles, brackets, and headlamp and mirror housings ▪ Electrical applications for connectors and fuses (Modern Plastics and Charles A. Harper 1999)

3.3.3 Nanosilicates: Clays and Colloidal Solids

Nanosilicate clays and colloidal solids may be relevant considerations for alternative flame retardant formulations. The DfE Hazard Evaluation Criteria cannot yet be applied to evaluation of nanomaterials. EPA does not have sufficient experience to apply data from one form of a chemical substance (such as a bulk material) to a particular nanoform of that chemical. Nanomaterials are not assessed in this report but they are still of interest to the partnership and this section provides a brief overview, including applications and available hazard information on two relevant example materials: organoclays and mesoporous silicate particles (MSPs). The information in this section is not intended to be comprehensive but is rather a starting point to help the reader conduct further research. Additional books and peer-reviewed publication references on nanosilicate flame retardants are provided in Appendix A.

Organoclays

Organoclays were developed in the 1930s and 1940s (Theng 1974) and were originally used as rheological modifiers, additives used to thicken coating materials. They have since been modified and Cloisite organoclays are now designed for use in plastics and rubbers for applications including flame retardant synergists. The use of bentonite (Mehta and Weiss 1978) and organoclays (Jonas 1970; Breitenfellner and Kainmülle 1985; Shain 1987) as additives to flame retardant formulations is claimed in several older patents; just over ten years ago Gilman, Kashiwagi and Lichtenhan (1997) published a paper on "Nanocomposites as a revolutionary new flame retardant approach." However, in the years that followed, it was discovered that adding organoclays to materials does not, by itself, enable materials to pass flame tests (Morgan 2006; Morgan and Wilke 2007). Organoclays improve flame retardant performance through synergistic actions, which has been documented for a variety of flame retardant additive types. When burned, organoclay particles in a nanocomposite move to the surface of the specimen increasing char strength and serving as a drip suppressant through formation of an insulating layer that can delay gasification. The typical loading amount varies between approximately three and six percent by weight (Gilman 1999; Gilman, Jackson et al. 2000)

Organoclays may pose a hazard to human health (minimal to moderate eye irritation, respiratory irritation observed in acute studies using high exposure levels, potential carcinogenicity) (US/International Council of Chemical Associations (ICCA) 2007), but the Organisation of Economic Cooperation and Development (OECD) has determined that organoclays are "of low priority for further work" (US/ICCA 2007).

Mesoporous silicate particles

MSPs can be thought of as holey silica 'beads.' Due to the large size of the pores, polymers interact with both the internal surfaces of the pores and the external surfaces of the particle, thereby forming a physically cross-linked polymer-particle network. The network created by the MSP provides a char barrier during combustion that reduces flame intensity while simultaneously improving the mechanical performance of the polymer into which they are compounded. (Some MSPs have surface areas in the range 200 to 1,200 m^2/g, uniform pores in the mesometric size range of 2 to 50 nm, and pore volumes between 0.20 and 2.0 cm^3/g (Pinnavaia, Roston et al. 2011)). As with organoclays, MSPs on their own will not typically

result in achieving flame retardancy, but by replacing a portion of the flame retardant loading with about 2 to 8 percent by weight MSPs, flame retardancy may be reached (Roston 2011).

Some MSP materials have been tested in various thermosets (e.g., glassy epoxy and polyester), and thermoplastics (e.g., PP, PE, and nylon 6) to assess their effectiveness as both a flame retardant agent and mechanical reinforcing agent. Some particles have demonstrated the ability to reduce fire intensity while simultaneously increasing the strength of the composite (Pinnavaia, Roston et al. 2011). Test results have also shown a reduction in dripping during fires (Pinnavaia, Roston et al. 2011). Manufacturer brochures state that their MSPs are low-toxicity submicron inorganic compositions that can be easily dispersed in a polymer matrix without the use of organic surface modification (University of California, Los Angeles (UCLA) 2009).

3.4 Flame Retardant Modes of Action

Polymer combustion is a complex process involving a number of interrelated and interdependent stages. It is possible to decrease the overall rate of polymer combustion by interfering with one or more of these stages. The basic mechanisms of flame retardancy will vary depending on the flame retardant and polymer system. Flame retardants can be classified based on the phase (solid or gas) in which they act to reduce or prevent propagation of flame. Other flame retardants may form protective barriers over a polymer which may insulate the flammable polymer from heat or reduce the amount of polymer that is available to burn as fuel.

3.4.1 Chemical Action in Condensed and Gas Phases

During fire, significant polymer degradation can occur due to heat in the condensed phase (1 mm from the flame/polymer interface), giving rise to volatile species that are liberated into the gas phase of the flame. Flame retardant compositions can either act on the condensed phase or the gas phase.

Radical Scavengers in the Gas Phase

Radical scavengers are also classified as chemical action flame retardant additives as they modify the radical process in the gas phase through chemical interaction with highly reactive species.

Halogenated Flame Retardants:

Halogenated flame retardants (e.g., decaBDE) mainly work through this mode of action by interfering with the gas phase of the combustion process (Troitzsch 1998). The mechanism of action of these types of flame retardants is shown in Figure 3-1. First, the flame retardant material breaks down and releases halogen radicals ($X^{\bullet}$) that react with the polymeric material (RH). The resulting reaction forms the corresponding halide (HX). The highly reactive radicals, hydrogen ($H^{\bullet}$) and hydroxyl ($OH^{\bullet}$), are responsible for degradation of volatile polymeric species into low molecular weight fragments. These radicals react with HX to produce less reactive (more stable) species, in some cases water, as shown in Figure 3-1. The addition of a catalytic amount of HX reduces the overall rate of combustion in this chain reaction (Hastie 1973). Consequently, the heat release rate and the heat transferred to the polymer are also reduced.

When the gas phase is saturated with less reactive radicals or species, the conditions for limiting combustion can be reached, thus extinguishing the flame.

Figure 3-1: Mechanism of action of halogenated flame retardant

$$X^{\bullet} + RH \rightarrow R^{\bullet} + HX$$
$$HX + H^{\bullet} \rightarrow H_2 + X^{\bullet}$$
$$HX + OH^{\bullet} \rightarrow H_2O + X^{\bullet}$$

Many aliphatic and aromatic halogenated flame retardants have been developed to meet specific compatibility requirements with commercial plastics. Brominated flame retardants are the preferred choice of halogenated flame retardants due to their cost effectiveness, effectiveness at low loading levels, and ease of processing (minimal/no detrimental effect on polymer processing).

Intumescents, Organic Char Forming Compounds and Radical Scavengers in the Condensed Phase

In the condensed phase, flame retardants can form protective barriers, which may be through intumescence or char formation, to prevent the propagation of flames. Phosphorous-based (e.g., ammonium polyphosphate, melamine polyphosphate) and nitrogen-based (e.g., melamine cyanurate) flame retardants both act in this way.

Some flame retardants cover the flammable polymer surface with a non-flammable protective coating. This helps insulate the polymer from the source of heat, reducing the formation of combustible breakdown products and release to the gas phase. The non-flammable coating may also prevent gaseous oxidants (e.g., oxygen from the air) from contacting the polymer surface. Intumescent compounds, which swell as a result of heat exposure, lead to the formation of a protective barrier in which the gaseous products of polymer decomposition are trapped.

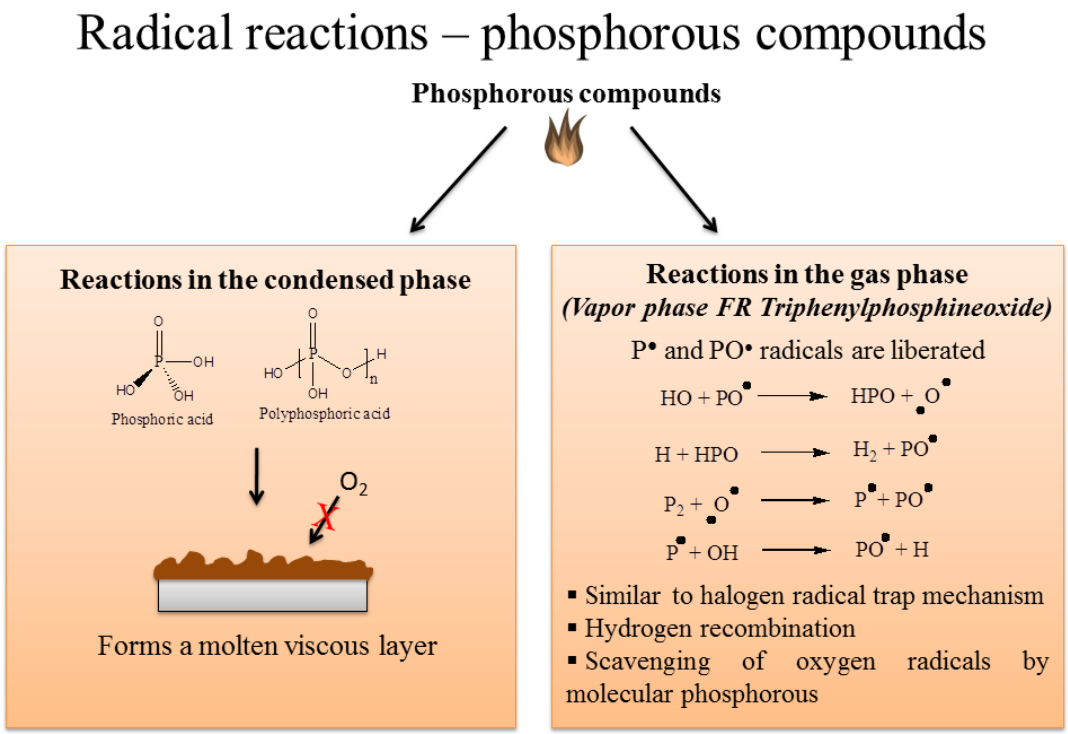
Alternatively, a non-flammable layer can be directly applied to the surface of the polymer to form a non-intumescent barrier coating. The formation of a thermally insulating char layer significantly influences subsequent degradation by serving as a protective coating layer preventing oxygen supply to the condensed phase. The properties of the char layer can further be bolstered by the presence of inorganic compounds. Many phosphorus-containing compounds form such non-intumescent surface chars. Char formation has several roles in flame retarding action. Char formation during combustion is an energy intensive process and occurs at the expense of other undesirable degradation reactions. There is dilution of the flame zone, and reduction in the amount of fuel available for further degradation (Kuryla 1979).

As mentioned above, both phosphorous- and nitrogen-based flame retardants work in the condensed phase. Below is a discussion on the modes of actions for these flame retardants.

Phosphorous Based Flame Retardants:

Phosphorous based flame retardants work efficiently in the condensed phase during combustion of a polymer. When heated, phosphorous reacts to produce phosphoric acid derivatives as shown in Figure 3-2. This acid is responsible for the formation of a glassy layer, which prevents flame propagation. Phosphorous-based flame retardants also generate intumescent char which acts as a two way barrier, namely hindering passage of combustible gas from the polymer to the flame and shielding the polymer layer from the flame. A range of phosphorous-based compounds including phosphines, phosphine oxides, phosphonium compounds, phosphonates, phosphinates, elemental red phosphorus, phosphites and phosphates are used as flame retardant additives. Phosphorus based flame retardants also include ammonium polyphosphate, melamine polyphosphate, and phosphate esters. Even though their predominant mode of action is through physical action (charring), there are certain proposed radical reactions that can take place during the combustion process as shown in Figure 3-2 (Carnaham, Haaf et al. 1979).

Figure 3-2: Mechanisms of flame retardant action in phosphorous based flame retardants



Source: Carnaham, Haaf et al. 1979

Inorganic phosphorus compounds are primarily used in PAs and phenolic resins, or as components in intumescent formulations. In the case of an intumescent material, a foamed char is developed on the surface upon combustion. In addition to char, intumescent materials can adhere to molten polymer, and help prevent dripping, which is necessary in fire quenching.

Nitrogen Based Flame Retardants:

Nitrogen-based compounds are often intumescent and were originally used in nitrogen-containing polymers such as polyurethanes and PAs. Melamine, melamine cyanurate, other melamine salts and guanidine compounds are currently the most used group of nitrogen-containing flame retardants. Melamine is used as a flame retardant additive for PP and PE. Melamine cyanurate is used as a flame retardant for PAs and polyesters (PET/PBT), epoxies and polyurethane resins. Melamine phosphate is also used in polyesters (PET/PBT).

3.4.2 Fillers / Diluents

Another mode of action is that exerted by inert solids incorporated into polymers. Such materials are known as fillers. Fillers include minerals like calcium carbonate or wollastonite. Sometimes the term filler gets used with magnesium and aluminum hydroxides due to their mineral structure. These mineral hydroxide fillers that impart flame retardant properties can be categorized as functional fillers. Metal hydroxides decompose with endothermicity when exposed to a fire and dilute the condensed phase of the burning polymer. These additives act as a heat sink, releasing water and/or carbon monoxide that interfere with combustion products in the vapor phase. As a result, fillers keep polymers cool and prevent them from thermally decomposing. Since fillers act predominantly via a physical rather than a chemical process, large loadings of fillers are needed to meet flammability standards.

3.4.3 Inorganic and Hydrated Compounds and Synergists

Metal hydroxides are the largest (by tonnage) class of all flame retardants used commercially and are employed alone or in combination with other flame retardants to achieve necessary improvements in flame retardancy. Metal hydroxides can function both in the condensed and gas phases of a fire by absorbing heat and decomposing to release their water. This process cools both the polymer and the flame and dilutes the flammable gas mixture. The high concentrations (typically 13 to 60 percent or greater by weight) required to impart flame retardants properties often adversely affect the mechanical properties of the polymer into which they are incorporated.

Aluminum hydroxide, also known as alumina trihydrate, is the largest volume flame retardant in use today. The low decomposition temperature (220-230°C), limits the polymers in which it can be incorporated. Magnesium hydroxide is stable to temperatures above 330-350°C and can be processed into several polymers.

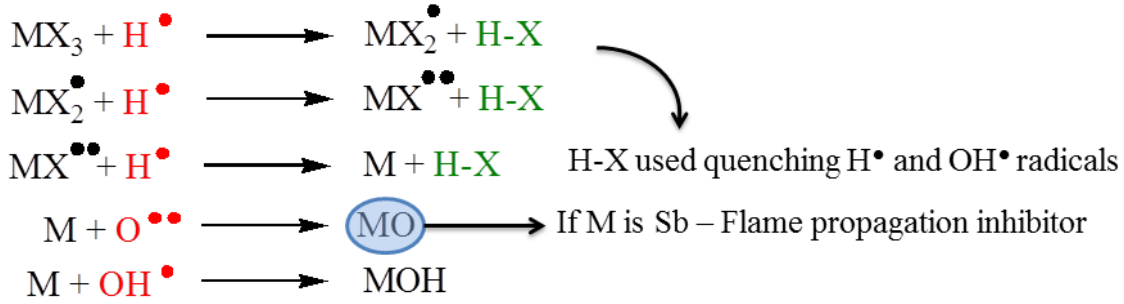
Antimony trioxide may not be considered a flame retardant by itself but is often used as a synergist. It is used in plastics, rubbers, textiles, paper and paints with organochlorine and organobromine compounds to diminish the flammability of a wide range of plastics and textiles. Boron compounds display synergism with antimony oxide. Zinc borate can function as a flame retardant and smoke suppressant.

Antimony-based compounds are synergistic co-additives used in combination with halogenated flame retardants, facilitating the reduction in total amount of flame retardants required to achieve a desired level of flame retardancy. Antimony oxides and antimonates are converted to volatile species by halogen acids in the fire. The halogen acids react with the antimony-containing

materials to form antimony trihalide and/or antimony halide oxide. The higher molecular weights of antimony halides in comparison to hydrogen halides, allow them to remain in the combustion zone longer, thus improving the efficiency of flame retardancy. This synergism only occurs in the presence of halogen flame retardants, as antimony does not react to form any other species in the presence of non-halogenated flame retardants.

Antimony oxychloride or trichloride reduces the rate at which the halogen leaves the flame zone, thus increasing the probability of reaction with the reactive species (i.e., hydroxyl radicals). The mechanism of action also involves radical scavenging as shown in Figure 3-3.

Figure 3-3: Synergistic Mechanism of Metal Halides Produced by a Combination of Halogen and Metal Oxides



Other Metal Based Compounds

Molybdenum compounds have been used as flame retardants in cellulosic materials and PVCs for many years and more recently with other polymers, mainly as smoke suppressants. Zinc compounds, such as zinc stannate and zinc hydroxy-stannate, are also used as synergists and as partial replacements for antimony trioxide.

3.4.4 Melting and Dripping

Some flame-retardant chemicals inhibit combustion by interfering with the transfer of heat from combustion back to the polymer (e.g., melamine cyanurate). Certain chemicals may promote depolymerization, which lowers the molecular weight of the polymer and facilitates melting. As the burning melt drips away from the bulk of the polymer it carries with it a proportion of the heat that would otherwise contribute to polymer decomposition and volatilization. By reducing the release of volatile decomposition products into the gas phase, these flame retardants reduce the amount of gaseous decomposition products available to feed the flame. While enhanced melting should decrease flammability in theory, in practice droplets of burning molten polymer may help spread a fire to other combustible materials.

3.4.5 Smoldering (Non-Flaming) Combustion

Smoldering (non-flaming) combustion and the closely related phenomenon of glowing combustion (i.e., only embers are present) occur primarily with high-surface area polymeric materials that break down during combustion to form a residual carbonaceous char (typically

cellulosic materials). In general, it is possible to inhibit non-flaming combustion either by retarding or preventing the initial breakdown of the polymer to form a char, or by interfering with the further combustion of this char. Boric acid and phosphates are the primary flame retardants used for preventing non-flaming combustion of organic polymers.

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4 Hazard Evaluation of DecaBDE and Alternatives

This chapter summarizes the toxicological and environmental hazards of decabromodiphenyl ether (decaBDE) and each alternative chemical that was identified as a potential functional substitute for decaBDE. In general, the hazard profiles include the assessment of unchanged starting materials, byproducts, and impurities. Evaluations of chemical formulations may also include associated substances if their presence is specifically required to allow that alternative to fully function in the assigned role. This report is a hazard assessment, not a risk assessment. Hazard assessment as a risk management tool is discussed in more detail in Section 1.4.

Toxicological and environmental endpoints included in the hazard profiles are discussed in Section 4.1 along with the criteria used to evaluate each hazard endpoint. Data sources and the review methodology are described in Section 4.2. The report then offers a detailed description of the utility of physical-chemical properties in understanding hazard in Section 4.3. Next, the process of evaluating human health and environmental endpoints are described in Sections 4.4 and 4.5, respectively and a discussion of the evaluation of endocrine activity is included in Section 4.6. The characteristics of each chemical included in the alternatives assessment are summarized in the comparative hazard summary table in Section 4.7. Lastly, the collected data and hazard profile of each chemical are presented in Section 4.8.

4.1 Toxicological and Environmental Endpoints

The assessment of endpoints with the intent to create hazard profiles for a Design for the Environment (DfE) alternatives assessment follows the guidance of the "Alternatives Assessment Criteria for Hazard Evaluation" (U.S. EPA 2011b). The definitions for each endpoint evaluated following these criteria are outlined in Section 4.1.1and the criteria by which these endpoints are evaluated are outlined in Section 4.1.2. Lastly, there are endpoints which DfE characterizes but does not assign criteria to and these are summarized in Section 4.1.3.

4.1.1 Definitions of Each Endpoint Evaluated Against Criteria

Hazard designations for each chemical discussed in this report were made by direct comparison of the experimental or estimated data to the DfE "Alternatives Assessment Criteria for Hazard Evaluation" (U.S. EPA 2011b). Table 4-1 provides a brief definition of human health toxicity, environmental toxicity and environmental fate endpoints.

Table 4-1: Definitions of Toxicological and Environmental Endpoints for Hazard Assessment

Endpoint Category	Endpoint	Definition
Human Health Effects	Acute mammalian toxicity	Adverse effects occurring following oral or dermal administration of a single dose of a substance, or multiple doses given within 24 hours, or an inhalation exposure of 4 hours.
	Carcinogenicity	Capability of a substance to increase the incidence of malignant neoplasms, reducing their latency, or increasing their severity or multiplicity.
	Mutagenicity/Genotoxicity	Mutagenicity - the ability of an agent to induce permanent, transmissible changes in the amount, chemical properties or structure of the genetic material. These changes may involve a single gene or gene segment, a block of genes, parts of chromosomes, or whole chromosomes. Mutagenicity differs from genotoxicity in that the change in the former case is transmissible to subsequent cell generations. Genotoxicity – the ability of an agent or processes to alter the structure, information content, or segregation of DNA, including those which cause DNA damage by interfering with normal replication process, or which in a non-physiological manner (temporarily) alter its replication.
	Reproductive toxicity	The occurrence of biologically adverse effects on the reproductive systems of females or males that may result from exposure to environmental agents. The toxicity may be expressed as alterations to the female or male reproductive organs, the related endocrine system, or pregnancy outcomes. The manifestation of such toxicity may include, but not limited to, adverse effects on onset of puberty, gamete production and transport, reproductive cycle normality, sexual behavior, fertility, gestation, parturition, lactation, developmental toxicity, premature reproductive senescence, or modifications in other functions that were dependent on the integrity of the reproductive systems.
	Developmental toxicity	Adverse effects in the developing organism that may result from exposure prior to conception (either parent), during prenatal development, or postnatally to the time of sexual maturation. Adverse developmental effects may be detected at any point in the lifespan of the organism. The major manifestations of developmental toxicity include: (1) death of the developing organism, (2) structural abnormality, (3) altered growth, and (4) functional deficiency.
	Neurotoxicity	An adverse change in the structure or function of the central and/or peripheral nervous system following exposure to a chemical, physical, or biological agent.

Endpoint Category	Endpoint	Definition
	Repeated dose toxicity	Adverse effects (immediate or delayed) that impair normal physiological function (reversible and irreversible) to specific target organs or biological systems following repeated exposure to a chemical substance by any route relevant to humans. Adverse effects include biologically significant changes in body and organ weights, changes that affect the function or morphology of tissues and organs (gross and microscopic), mortality, and changes in biochemistry, urinalysis, and hematology parameters that are relevant for human health; may also include immunological and neurological effects.
	Respiratory sensitization	Result of a substance that will lead to hypersensitivity of the airways following inhalation of the substance.
	Skin sensitization	A chemical that elicits a cell-mediated or antibody-mediated allergic response characterized by the presence of inflammation that may result in cell death, following an initial induction exposure to the same chemical substance, i.e., skin allergy.
	Eye irritation/corrosivity	Irritation or corrosion to the eye following the application of a test substance.
	Skin irritation/corrosion	Skin irritation is reversible damage to the skin following the application of a test substance for up to 4 hours. Skin corrosion is irreversible damage to the skin namely, visible necrosis through the epidermis and into the dermis following the application of a test substance for up to 4 hours.
Environmental Toxicity	Adverse effects observed in living organisms that typically inhabit the wild; the assessment is focused on effects in three groups of surrogate aquatic organisms (freshwater fish, invertebrates, and algae).	
	Aquatic toxicity (Acute)	The property of a substance to be injurious to an organism in a short-term, aquatic exposure to that substance.
	Aquatic toxicity (Chronic)	The property of a substance to cause adverse effects to aquatic organisms during aquatic exposures which were determined in relation to the life-cycle of the organism.
Environmental Fate	Environmental Persistence	The length of time the chemical exists in the environment, expressed as a half-life, before it is destroyed (i.e., transformed) by natural or chemical processes. For alternative assessments, the amount of time for complete assimilation (ultimate removal) is preferred over the initial step in the transformation (primary removal).

Endpoint Category	Endpoint	Definition
	Bioaccumulation	The process in which a chemical substance is absorbed in an organism by all routes of exposure as occurs in the natural environment, e.g., dietary and ambient environment sources. Bioaccumulation is the net result of competing processes of chemical uptake into the organism at the respiratory surface and from the diet and chemical elimination from the organism including respiratory exchange, fecal egestion, metabolic biotransformation of the parent compound and growth dilution.

The hazard profile for each chemical contains a summary statement (Section 4.8). For each of the endpoints in Table 4-1 the summary statement gives the hazard designation, the type of data (experimental or estimated), and the rationale. The endpoint summaries may also include explanatory comments, a discussion of confounding factors, or an indication of the confidence in the data to help put the results in perspective.

4.1.2 Criteria

Table 4-2 summarizes the criteria that were used by the U.S. Environmental Protection Agency (EPA) DfE Program to interpret the data presented in the hazard evaluations. The DfE Alternatives Assessment Criteria for Hazard Evaluation underwent internal and public comment, and were finalized in 2011 (U.S. EPA 2011b). A hazard designation for each human health endpoint was not given for each route of exposure but rather was based on the exposure route with the highest hazard designation. Data may have been available for some or all relevant routes of exposure.

The details as to how each endpoint was evaluated are described below and in the DfE full criteria document, DfE Alternatives Assessment Criteria for Hazard Evaluation, available at: http://www.epa.gov/dfe/alternatives_assessment_criteria_for_hazard_eval.pdf.

Table 4-2: Criteria Used to Assign Hazard Designations

Endpoint	Very High	High	Moderate	Low	Very Low
Human Health Effects					
Acute mammalian toxicity					
Oral median lethal dose (LD_{50}) (mg/kg)	≤50	>50–300	>300–2000	>2000	–
Dermal LD_{50} (mg/kg)	≤200	>200–1000	>1000–2000	>2000	–
Inhalation median lethal concentration (LC_{50}) - vapor/gas (mg/L)	≤2	>2–10	>10–20	>20	–
Inhalation LC_{50} - dust/mist/ fume (mg/L)	≤0.5	>0.5–1.0	>1–5	>5	–
Carcinogenicity					

Endpoint	Very High	High	Moderate	Low	Very Low
	Known or presumed human carcinogen (equivalent to Globally Harmonized System of Classification and Labeling of Chemicals (GHS) Category 1A and 1B)	Suspected human carcinogen (equivalent to GHS Category 2)	Limited or marginal evidence of carcinogenicity in animals (and inadequate evidence in humans)	Negative studies or robust mechanism-based SAR (as described above)	–
Mutagenicity/Genotoxicity					
Germ cell mutagenicity	GHS Category 1A or 1B: Substances known to induce heritable mutations or to be regarded as if they induce heritable mutations in the germ cells of humans	GHS Category 2: Substances which cause concern for humans owing to the possibility that they may induce heritable mutations in the germ cells of humans OR	Evidence of mutagenicity supported by positive results in *in vitro* OR *in vivo* somatic cells of humans or animals	Negative for chromosomal aberrations and gene mutations, or no structural alerts.	--
Mutagenicity and genotoxicity in somatic cells		Evidence of mutagenicity supported by positive results in *in vitro* AND *in vivo* somatic cells and/or germ cells of humans or animals			
Reproductive toxicity					
Oral (mg/kg/day)	–	<50	50–250	>250-1000	>1000
Dermal (mg/kg/day)	–	<100	100–500	>500-2000	>2000
Inhalation - vapor, gas (mg/L/day)	–	<1	1–2.5	>2.5-20	>20
Inhalation - dust/mist/fume (mg/L/day)	–	<0.1	0.1–0.5	>0.5-5	>5
Developmental toxicity					
Oral (mg/kg/day)	–	<50	50–250	>250-1000	>1000
Dermal (mg/kg/day)	–	<100	100–500	>500-2000	>2000
Inhalation - vapor, gas (mg/L/day)	–	<1	1–2.5	>2.5-20	>20

Endpoint	Very High	High	Moderate	Low	Very Low
Inhalation - dust/mist/fume (mg/L/day)	–	<0.1	0.1–0.5	>0.5-5	>5
Neurotoxicity					
Oral (mg/kg/day)	–	<10	10–100	>100	–
Dermal (mg/kg/day)	–	<20	20–200	>200	–
Inhalation - vapor, gas (mg/L/day)	–	<0.2	0.2–1.0	>1.0	–
Inhalation - dust/mist/fume (mg/L/day)	–	<0.02	0.02–0.2	>0.2	–
Repeated-dose toxicity					
Oral (mg/kg/day)	–	<10	10–100	>100	–
Dermal (mg/kg/day)	–	<20	20–200	>200	–
Inhalation - vapor, gas (mg/L/day)	–	<0.2	0.2–1.0	>1.0	–
Inhalation - dust/mist/fume (mg/L/day)	–	<0.02	0.02–0.2	>0.2	–
Sensitization					
Skin sensitization	–	High frequency of sensitization in humans and/or high potency in animals (GHS Category 1A)	Low to moderate frequency of sensitization in human and/or low to moderate potency in animals (GHS Category 1B)	Adequate data available and not GHS Category 1A or 1B	–
Respiratory sensitization	–	Occurrence in humans or evidence of sensitization in humans based on animal or other tests (equivalent to GHS Category 1A and 1B)	Limited evidence including the presence of structural alerts	Adequate data available indicating lack of respiratory sensitization	–
Irritation/corrosivity					
Eye irritation/corrosivity	Irritation persists for >21 days or corrosive	Clearing in 8–21 days, severely irritating	Clearing in ≤7 days, moderately irritating	Clearing in <24 hours, mildly irritating	Not irritating
Skin irritation/corrosivity	Corrosive	Severe irritation at 72 hours	Moderate irritation at 72 hours	Mild or slight irritation at 72 hours	Not irritating
Endocrine activity					
	For this endpoint, High/Moderate/Low etc. characterizations will not apply. A qualitative assessment of available data will be prepared.				
Environmental Toxicity and Fate					
Aquatic toxicity					

Endpoint	Very High	High	Moderate	Low	Very Low
Acute aquatic toxicity - LC_{50} or half maximal effective concentration (EC_{50}) (mg/L)	<1.0	1–10	>10–100	>100 or No Effects at Saturation (NES)	–
Chronic aquatic toxicity – lowest observed effect concentration (LOEC) or chronic value (ChV) (mg/L)	<0.1	0.1–1	>1–10	>10 or NES	–
Environmental persistence					
Persistence in water, soil, or sediment	Half-life >180 days or recalcitrant	Half-life of 60–180 days	Half-life <60 but ≥16 days	Half-life <16 days OR passes Ready Biodegradability test not including the 10-day window. No degradation products of concern.	Passes Ready Biodegradability test with 10-day window. No degradation products of concern.
Persistence in air (half-life days)	For this endpoint, High/Moderate/Low etc. characterizations will not apply. A qualitative assessment of available data will be prepared.				
Bioaccumulation					
Bioconcentration Factor (BCF)/Bioaccumulation Factor (BAF)	>5000	5000–1000	<1000–100	<100	–
Log BCF/BAF	>3.7	3.7–3	<3-2	<2	–

Very High or Very Low designations (if an option for a given endpoint in Table 4-2) were assigned only when there were experimental data located for the chemical under evaluation. In addition, the experimental data must have been collected from a well conducted study specifically designed to evaluate the endpoint under review. If the endpoint was estimated using experimental data from a close structural analog, by professional judgment, or from a computerized model, then the next-level designation was assigned (e.g., use of data from a structural analog that would yield a designation of very high would result in a designation of high for the chemical in review). One exception is for the estimated persistence of polymers with an average molecular weight >1,000, which may result in a Very High designation.

4.1.3 Endpoints Characterized but Not Evaluated

Several additional endpoints were characterized, but not evaluated against hazard criteria. This is because the endpoints lacked a clear consensus concerning the evaluation criteria (endocrine activity), data and expert judgment were limited for industrial chemicals (persistence in air, terrestrial ecotoxicology), or the information was valuable for the interpretation of other toxicity and fate endpoints (including toxicokinetics and transport in the environment).

Table 4-3: Definitions of Endpoints and Information Characterized but Not Evaluated Against Hazard Criteria

Toxicological Endpoint	Definition
Toxicokinetics	The determination and quantification of the time course of absorption, distribution, biotransformation, and excretion of chemicals (sometimes referred to as pharmacokinetics).
Biomonitoring Information	The measured concentration of a chemical in biological tissues where the analysis samples were obtained from a natural or non-experimental setting.
Environmental Transport	The potential movement of a chemical, after it is released to the environment, within and between each of the environmental compartments, air, water, soil, and sediment. Presented as a qualitative summary in the alternative assessment based on physical-chemical properties, environmental fate parameters, and simple volatilization models. Also includes distribution in the environment as estimated from a fugacity model.
Persistence in Air	The half-life for destructive removal of a chemical substance in the atmosphere. The primary chemical reactions considered for atmospheric persistence include hydrolysis, direct photolysis, and the gas phase reaction with hydroxyl radicals, ozone, or nitrate radicals. Results are used as input into the environmental transport models.
Immunotoxicology	Adverse effects on the normal structure or function of the immune system caused by chemical substances (gross and microscopic changes to immune system organs, suppression of immunological response, autoimmunity, hypersensitivity, inflammation, and disruption of immunological mechanistic pathways).
Terrestrial Ecotoxicology	Reported experimental values effects from guideline and nonguideline studies on adverse effects on the terrestrial environment. Studies on soil, plants, birds, mammals, invertebrates were also included.
Endocrine Activity	A change in endocrine homeostasis caused by a chemical or other stressor from human activities (e.g., application of pesticides, the discharge of industrial chemicals to air, land, or water, or the use of synthetic chemicals in consumer products.)

4.2 Data Sources and Assessment Methodology

This section explains how data were collected (Section 4.2.1), prioritized and reviewed (Section 4.2.2) for use in the development of hazard profiles. High-quality experimental studies lead to a thorough understanding of behavior and effects of the chemical in environment and in living organisms. Analog approaches and SAR-based estimation methods are also useful tools and are discussed throughout this Section. Information on how polymers differ from discrete chemicals in terms of how they are evaluated is presented in Section 4.2.3.

4.2.1 Identifying and Reviewing Measured Data

For each chemical assessed, data were collected in a manner consistent with the HPV Chemical Challenge Program guidance (U.S. EPA 1999b) on searching for existing chemical information. This process resulted in a comprehensive search of the literature for available experimental data. For well characterized chemicals this usually resulted in the collection of recent high-quality reviews or peer-reviewed risk assessments. These were supplemented by primary searches of scientific literature published after these secondary sources were released, this explained in

greater detail below. For chemicals that are not as well characterized, that is, where these secondary sources were not available or lacked relevant or adequate data, a comprehensive search of the primary scientific literature was done. Subsequently, these searches led to the collection and review of articles from the scientific literature, industrial submissions, encyclopedic sources, and government reports. In addition, data presented in U.S. EPA public and confidential databases (e.g., integrated risk information system (IRIS)) were obtained for this project. Generally, foreign language (non-English) reports were not used unless they provided information that was not available from other sources.

Chemical assessments were performed by first searching for experimental data for all endpoints in Table 4-2. For most chemicals assessed, high quality secondary sources were not available to assess all endpoints, and a comprehensive search of the literature was performed to identify experimental data. In some cases, confidential studies submitted to EPA by chemical manufacturers were also available to support hazard designations. For those chemicals that were expected to form stable metabolites, searches were performed to identify relevant fate and toxicity information for the metabolite or degradate.

Well Studied Chemicals – Literature Search Strategy

As mentioned above, for chemicals that have been well studied, the literature review focused primarily on the use of secondary sources, such as Agency for Toxic Substances and Disease Registry Toxicological Profiles or IRIS assessments. Using high-quality secondary sources maximized available resources and eliminated potential duplication of effort. However, more than one secondary source was typically used to verify reported values, which also reduced the potential for presenting a value that was transcribed incorrectly from the scientific literature. Although other sources might also contain the same experimental value for an endpoint, effort was not focused on building a comprehensive list of these references, as it would not have enhanced the ability to reach a conclusion in the assessment. When data for a selected endpoint could not be located in a secondary source for an otherwise well-studied chemical, the primary literature was searched by endpoint and experimental studies were assessed for relevant information.

Making Predictions in the Absence of Measured Data

In the absence of primary or secondary data, hazard designations were based on (1) Quantitative Structure Activity Relationships (QSAR)-based estimations from the EPA New Chemical Program's predictive methods; (2) analog data (3) class-based assignments from the EPA Chemical Categories document; and (4) expert judgment by EPA subject matter experts.

For chemicals that lacked experimental information, QSAR assessments were made using either EPA's Estimation Programs Interface (EPISuite^{TM}) for physical-chemical property and environmental fate endpoints or EPA's Ecological Structure Activity Relationships (ECOSAR^{TM}) QSARs for ecotoxicity. For the cancer endpoint, estimates were also obtained from EPA's OncoLogic expert system. These estimation methods have been automated, and are available for free (U.S. EPA 2012c). Often analog data were used to support predictions from

models. These approaches were described in the EPA Pollution Prevention (P2) Framework and Sustainable Futures (SF) program (U.S. EPA 2005c; U.S. EPA 2011e).

For some physical-chemical properties that could not be estimated using EPISuite™, such as acid/base dissociation constants, other available methods (e.g., the Sparc website for dissociation constants) were used. All estimation methods employed were limited to those freely available in the public domain.

The methodology and procedures used to assess polymers are described in Section 4.2.3. In addition, the endpoints for impurities or oligomers with a molecular weight (MW) >1,000 were estimated using professional judgment and the results assessed for inclusion in the overall hazard designation. This process is described, as appropriate, under the corresponding endpoints appearing in Section 4.3.

When QSAR models were not available, professional judgment was used to identify hazards for similar chemicals using the guidance from EPA's New Chemicals Categories (U.S. EPA 2010g). The categories identify substances that share chemical and toxicological properties and possess potential health or environmental concerns (U.S. EPA 2010a). In the absence of an identified category, analogs for which experimental data are available were identified using EPA's Analog Identification Methodology (AIM) or by substructure searches of confidential EPA databases (U.S. EPA 2012a). If a hazard designation was still not available, the expert judgment of scientists from EPA's New Chemical Program would provide an assessment of the physical-chemical properties, environmental fate, aquatic toxicity, and human health endpoints to fill remaining data gaps.

4.2.2 Hierarchy of Data Adequacy

Once the studies were obtained they were then evaluated to establish whether the hazard data were of sufficient quality to meet the requirements of the assessment process. The adequacy and quality of the studies identified in the literature review are described in the Data Quality field of the chemical assessments presented in Section 4.8. The tiered approach described below represents a general preferred data hierarchy, but the evaluation of toxicological data also requires flexibility based on expert judgment.

1. One or more studies conducted in a manner consistent with established testing guidelines
2. Experimentally valid but nonguideline studies (i.e., do not follow established testing guidelines)
3. Reported data without supporting experimental details
4. Estimated data using SAR methods or professional judgment based on an analog approach
5. Expert judgment based on mechanistic and structural considerations

In general, data were considered adequate to characterize an endpoint if they were obtained using the techniques identified in the High Production Volume (HPV) data adequacy guidelines (U.S. EPA 1999b). Studies performed according to Harmonized EPA or Organisation for Economic

Cooperation and Development guidelines were reviewed to confirm that the studies followed all required steps.

Experimental studies published in the open literature were reviewed for their scientific rigor and were also compared and contrasted to guideline studies to identify potential problems arising from differences in the experimental design. Data from adequate, well-performed, experimental studies were used to assign hazard designations in preference to those lacking in sufficient experimental detail. When multiple adequate studies were available for a given endpoint, any conflicts that were identified were addressed using a weight-of-evidence approach to characterize the endpoint whenever possible.

When available, experimental data from guideline or well-performed experimental studies were preferred (items 1 and 2 in the hierarchy list). Information from secondary sources such as Material Safety Data Sheets, or online databases (such as the National Library of Medicine's Hazardous Substances Data Bank) (item 3 in the hierarchy list) was considered appropriate for some endpoints when it included numerical values for effect levels that could be compared to the evaluation criteria.

4.2.3 Assessment of Polymers and Oligomers

The methodology and procedures used to assess polymers was slightly different than that used for oligomers, discrete compounds and simple mixtures. Although experimental data for polymers were identified using the literature search techniques discussed above in Section 4.2.1, in the absence of experimental data, estimates were performed using professional judgment as presented in the SF Polymer Assessment guidance (U.S. EPA 2010d). The polymers are a mixture of molecules with a distribution of components (e.g. different chain lengths) that depend on the monomers used, their molar ratios, the total number of monomeric units in the polymer chain, and the manufacturing conditions. To account for this variation, the average MW profile (also referred to as the number average molecular weight MW_n) was used in their assessment as the individual chains rarely have the same degree of polymerization and weight yet their physical, chemical, and environmental properties are essentially identical for the purposes of this assessment. The polymers evaluated as alternatives typically have average MWs ranging from >1,000 to <100,000 daltons.

For polymers with relatively low average MWs (i.e., those with average MWs generally less than 2,000), the alternative assessment also determined the amount of oligomers and unchanged monomers (starting materials) in the MW profile with MWs <1,000 daltons. Special attention was paid to materials that have a MW <1,000 daltons as these materials often have the highest hazard (potentially bioavailable substances) in the mixture. This type of assessment was similar to the evaluation of the hazards of impurities present in discrete chemical products. Methodological differences between the evaluation of discrete products and polymers are discussed in Section 4.3.

For the Alternatives Assessment, there were chemicals that are mixtures of low MW oligomers comprised of 2 or 3 repeating units. The hazard assessment evaluated all oligomers present. From all the oligomers, the higher concern material was used to assign the hazard designation. This process is essentially identical to the evaluation of the hazards associated with impurities or

byproducts present in discrete chemical products. As a result, the alternatives assessment process determined the amount of oligomers and unchanged monomers (starting materials) present and considered their potential hazards in the alternatives designation.

4.3 Importance of Physical and Chemical Properties, Environmental Transport, and Biodegradation

Physical-chemical properties provide basic information on the characteristics of a chemical substance and were used throughout the alternatives assessment process. These endpoints provide information required to assess potential environmental release, exposure, and partitioning as well as insight into the potential for adverse toxicological effects. The physical-chemical properties are given in the individual chemical hazard profiles presented in Section 4.8. For information on how key physical-chemical properties of alternatives can be used to address the potential for human and environmental exposure, please refer to Table 5-1. Descriptions of relevant physical-chemical properties and how they contribute to the hazard assessments are presented below.

Molecular Weight (MW)

MW informs how a chemical behaves in a physical or biological system including bioavailability and environmental fate. In general, but not strictly, larger compounds tend to be less mobile in biological and environmental systems. Their large size restricts their transport through biological membranes and lowers their vapor pressure. Polymers and oligomers evaluated in this alternatives assessment were mixtures that contain a distribution of components and they may not have a unique MW (see also Section 4.2.3). To account for variation in these mixtures, the average MW or MW_n, determined experimentally (typically using high pressure liquid chromatography, viscosity, or light-scattering), was used in the assessment of polymers. The assessment of polymers also includes oligomers and unchanged monomers (starting materials) that have MW of <1,000 daltons as these were often the highest concern materials (bioavailable substances) in the mixture.

Melting Point and Boiling Point

These two properties provide an indication of the physical state of the material at ambient temperature. Chemicals with a melting point more than 25°C were assessed as a solid. Those with a melting point less than 25°C and a boiling point more than 25°C were assessed as a liquid and those with a boiling point less than 25°C were assessed as a gas. The physical state was used throughout the assessment, such as in the determination of potential routes of human and environmental exposure, as described in Section 5.2. The melting and boiling points were also useful in determining the potential environmental fate, ecotoxicity, and human health hazards of a chemical. For example, organic compounds with high melting points generally have low water solubility and low rates of dissolution. These properties influence a material's bioavailability and were therefore taken into account in both the assessment process and the evaluation of experimental studies. Similarly, chemicals with a low melting point also have a higher potential to be absorbed through the skin, gastrointestinal tract, and lungs.

In the absence of experimental data, the melting point value was not reported and no estimations were performed. If a chemical decomposes before it melts, this information was included in the

assessment. For boiling point, the maximum value reported in the assessment was 300°C for high boiling materials including polymers (U.S. EPA 1999b). Melting points for polymers and/or oligomers were not reported as these materials typically reach a softening point and do not undergo the phase change associated with melting (i.e., solid to liquid).

Vapor Pressure

Vapor pressure is useful in determining the potential for a chemical substance to volatilize to the atmosphere from dry surfaces, from storage containers, or during mixing, transfer, or loading/unloading operations (see Section 5.2). In the assessment process, chemicals with a vapor pressure less than 1×10^{-6} mm Hg have a low potential for inhalation exposure resulting from gases or vapors. Vapor pressure is also useful for determining the potential environmental fate of a substance. Substances with a vapor pressure more than 1×10^{-4} mm Hg generally exist in the gas phase in the atmosphere. Substances with a vapor pressure between 1×10^{-4} and 1×10^{-8} mm Hg exist as a gas/particulate mixture. Substances with a vapor pressure less than 1×10^{-8} mm Hg exist as a particulate. The potential atmospheric degradation processes described below in the reactivity section generally occur when a chemical exists in the gas phase. Gases in the atmosphere also have the potential to travel long distances from their original point of release. Materials in the liquid or solid (particulate) phases in the atmosphere generally undergo deposition onto the Earth's surface.

A maximum vapor pressure of 1×10^{-8} mm Hg was assigned for chemicals without experimental data or for those substances that were anticipated by professional judgment to be nonvolatile (U.S. EPA 2011e). The maximum vapor pressure of 1×10^{-8} mm Hg was also the default value reported for the vapor pressure of polymers with a MW >1,000 daltons (U.S. EPA 2010d).

Water Solubility

The water solubility of a chemical provides an indication of its distribution between environmental media, potential for environmental exposure through release to aquatic compartments, and potential for human exposure through ingestion of drinking water; water solubility was also used extensively to determine potential human health and ecotoxicity hazards. In general, chemicals with water solubility less than 1×10^{-5} g/L indicate a lower concern for both the expression of adverse effects, and potential aquatic and general population exposure due to their low bioavailability. However, chemicals with a low bioavailability also tend to be more environmentally persistent. Low bioavailability is different than no bioavailability, and the two should not be used interchangeably.

Within the context of this alternatives assessment, the following descriptors were used according to ranges of water solubility values: more than 10,000 mg/L was considered very soluble; 1,000–10,000 mg/L represents soluble; 100–1,000 mg/L represents moderately soluble, 1–100 mg/L represents slightly soluble, and less than 1 mg/L represents insoluble, noting that these guidelines were not followed consistently within the scientific literature (U.S. EPA 2011e). Chemicals with higher water solubility were more likely to be transported into groundwater with runoff during storm events, be absorbed through the gastrointestinal tract or lungs, partition to aquatic compartments, undergo atmospheric removal by rain washout, and possess a greater potential for

human exposure through the ingestion of contaminated drinking water. Chemicals with lower water solubility were generally more persistent and have a greater potential to bioconcentrate.

The water solubility of a substance was also used to evaluate the quality of experimental aquatic toxicity and oral exposure human health studies as well as the reliability of aquatic toxicity estimates. If the water solubility of a substance was lower than the reported exposure level in these experiments, then the study was likely to be regarded as inadequate due to potentially confounding factors arising from the presence of un-dissolved material. For aquatic toxicity estimates obtained using SARs, when the estimated toxicity was higher than a chemical's water solubility (i.e., the estimated concentration in water at which adverse effects appear cannot be reached because it was above the material's water solubility), the chemical was described as having NES. When NES occurs, a low ecotoxicity hazard designation was assigned.

While assessing the water solubility of a chemical substance, its potential to disperse in an aqueous solution was also considered. Ideally, a chemicals potential to disperse would be obtained from the scientific literature. In the absence of experimental data, the potential for dispersion can be determined from chemical structure and/or comparison to closely related analogs. There are two general structural characteristics that lead to the formation of dispersions in water: (1) chemicals that have both a hydrophilic (polar) head and a hydrophobic (nonpolar) tail (e.g., surfactants), and (2) molecules that have a large number of repeating polar functional groups (e.g., polyethylene oxide).

The potential for a chemical to disperse influences potential exposure, environmental fate, and toxicity. Dispersible chemicals have greater potential for human and environmental exposure, leachability, and aquatic toxicity than what might be anticipated based on the material's water solubility alone.

Chemicals without experimental data or chemicals that were anticipated by professional judgment to be sufficiently insoluble and thus were not bioavailable were assigned a water solubility maximum value of 1×10^{-3} mg/L (U.S. EPA 2011e). A water solubility of 1×10^{-3} mg/L is the default value used for discrete organics as well as non-ionic polymers with a MW > 1,000 daltons according to SF Polymer Assessment guidance (U.S. EPA 2010d). This assignment is consistent with an analysis of the chemicals used in the development of the water solubility estimation program in EPA's EPISuite™ software. The training set for this model included 1,450 chemicals with a MW range 27-628 daltons and experimental water solubilities ranging from miscible to 4×10^{-7} mg/L (Meylan, Howard et al. 1996; U.S. EPA 2011i). Given that water solubility decreases with MW, a default value of 1×10^{-3} mg/L is consistent with the limited bioavailability expected for materials with a MW >1,000 daltons.

Octanol/Water Partition Coefficient (K_{ow})

The octanol/water partition coefficient, commonly expressed as its log value (i.e., log K_{ow}) is one of the most useful properties for performing a hazard assessment. The log K_{ow} provides the partitioning between octanol and water, where octanol is used to mimic fat and other hydrophobic components of biological systems. Chemicals with a log K_{ow} less than 1 are highly soluble in water (hydrophilic), while those with a log K_{ow} more than 4 are not very soluble in

water (hydrophobic). A log K_{ow} more than 8 indicates that the chemical is not readily bioavailable and is essentially insoluble in water. In addition, log K_{ow}s greater than approximately 8 may be difficult to obtain experimentally.

The log K_{ow} can be used as a surrogate for the water solubility in a hazard assessment and is frequently used to estimate the water solubility if an experimental value is not available. It can also be used to estimate other properties important to the assessment, including bioconcentration and soil adsorption, and is a required input for SAR models used to estimate ecotoxicity values.

For chemicals without data, that are not within the domain of EPISuite™ or that were expected to be insoluble in water (WS <1 x 10^{-3} mg/L), a minimum value of 10 was assigned for the log K_{ow} (U.S. EPA 2011e). Insoluble chemicals that could be run through EPISuite™ software may use a log K_{ow} >10 if the result appeared to be valid based on expert review. This assignment is consistent with an analysis of the chemicals ("training set") used in the development of the octanol/water partition coefficient estimation program in the EPISuite™ software. The training set for this model included 10,946 chemicals with a MW range 18-720 daltons and experimental log K_{ow}s ranging from -3.89 to 8.70 (Meylan and Howard 1995; U.S. EPA 2011h). Given that log K_{ow} increases with MW, a default value of 10 is consistent with the limited bioavailability expected for materials with a MW >1,000 daltons. A maximum log K_{ow} of -2 was used for water soluble materials. For most polymers and other materials that are anticipated to be insoluble in both water and octanol, the log K_{ow} cannot be measured and was therefore not listed.

Flammability (Flash Point)

The flash point of a substance is defined as the minimum temperature at which the substance emits sufficient vapor to form an ignitable mixture with air. Flash point can be used to identify hazards associated with the handling of volatile chemicals. Substances with a flash point above 37.8°C (100°F) were commonly referred to as non-flammable, as this is the flammability definition used in the shipping industry. There are exceptions to this definition such as chemicals that may form explosive mixtures in the presence of air.

Explosivity

Explosivity refers to the potential for a chemical to form explosive mixtures in air and can be defined using the limits of flammability. The lower limit of flammability (LFL) is defined as the minimum concentration of a combustible substance that is capable of propagating a flame through a homogenous mixture in the presence of an ignition source. The upper limit of flammability (UFL) is similarly defined as the highest concentration that can propagate a flame. LFLs and UFLs are commonly reported as the volume percent or volume fraction of the flammable component in air at 25°C. If the ambient air concentration of the gas (or vapor) is between the upper and lower explosion limit, then the material has the potential to explode if it comes in contact with an ignition source. Knowledge regarding the explosivity of a given material in air is also useful in identifying potential hazards associated with the manufacture and use of that material.

pH

The pH scale measures how acidic or basic a substance is on a range from 0 to 14. A pH of 7 is neutral. A pH less than 7 is acidic, and a pH greater than 7 is basic. It is used primarily to identify potential hazards associated with skin or eye contact with a chemical or its aqueous solutions. The corrosive nature of chemicals that form either strongly basic (high pH) or strongly acidic (low pH) solutions are generally likely to result in harm to skin and other biological membranes. For corrosive chemicals, some experimental studies, such as biodegradation tests, require additional analysis to determine if the tests were performed at concentrations that cause harm to microbes in the test (and, therefore, may result in incorrectly identifying a chemical as persistent in the environment). For chemicals that form moderately basic or acidic solutions in water, the pH of the resulting solution can be used in lieu of a measured dissociation constant.

Dissociation Constant in Water (pKa)

The dissociation constant determines if a chemical will ionize under environmental conditions. The dissociation constant in water provides the amount of the dissociated and undissociated forms of an acid, base, or organic salt in water. Knowledge of the dissociation constant is required to assess the importance of the other physical-chemical properties used in the hazard assessment. As the percentage of ionization increases, the water solubility increases while the vapor pressure, Henry's Law constant, and octanol/water partition coefficient decrease. For acids and bases, the dissociation constant was expressed as the pK_A and pK_B, respectively.

Henry's Law Constant

Henry's Law constant is the ratio of a chemical's concentration in the gas phase to that in the liquid phase (at equilibrium). In environmental assessments, the Henry's Law constant is typically measured in water at 25°C. The Henry's Law constant provides an indication of a chemical's volatility from water, which can be used to derive partitioning within environmental compartments and the amount of material removed by stripping in a sewage treatment plant. Henry's Law constants less than 1×10^{-7} atm-m^3/mole indicate slow volatilization from water to air (the Henry's Law constant for the volatilization of water from water is 1×10^{-7} atm-m^3/mole) and values more than 1×10^{-3} atm-m^3/mole indicate rapid volatilization from water to air. To aid in determining the importance of volatilization, the assessment uses two models based on the Henry's Law constant. These models determine the half-life for volatilization from a model river and a model lake. A maximum value of 1×10^{-8} atm-m^3/mole for the Henry's Law Constant was assigned for chemicals without experimental data or for those that were anticipated by professional judgment to be nonvolatile.

Sediment/Soil Adsorption/Desorption Coefficient (K_{oc})

The soil adsorption coefficient provides a measure of a chemical's ability to adsorb to the organic portion of soil and sediment. This provides an indication of the potential for the chemical to leach through soil and be introduced into groundwater, which may lead to environmental exposures to wildlife or humans through the ingestion of drinking water drawn from underground sources. Chemicals with high soil adsorption coefficients are expected to be

strongly adsorbed to soil and are unlikely to leach into ground water. The soil adsorption coefficient also describes the potential for a chemical to partition from environmental waters to suspended solids and sediment. The higher the K_{oc} the more strongly a chemical is adsorbed to soil. Strong adsorption may impact other fate processes, such as the rate of biodegradation, by making the chemical less bioavailable.

The soil adsorption coefficient, K_{oc}, is normalized with respect to the organic carbon content of the soil to account for geographic differences. The assignments for the degree that a chemical is adsorbed to soil within the context of the assessment were described qualitatively as very strong (above 30,000), strong (above 3,000), moderate (above 300), low (above 30), and negligible (above 3). When determining the potential for a chemical to adsorb to soil and suspended organic matter, the potential for a chemical to form chemical bonds with humic acids and attach to soil also needs to be considered, although this process is generally limited to a small number of chemical classes.

A maximum value of 30,000 for the K_{oc} was assigned for chemicals without experimental data or for those that were anticipated by professional judgment to be strongly absorbed to soil (U.S. EPA 2011e). A default K_{oc} of 30,000 was used for polymers with a MW >1,000 daltons.

Reactivity

The potential for a substance to undergo irreversible chemical reactions in the environment can be used in the assessment of persistence. The primary chemical reactions considered in an environmental fate assessment are hydrolysis, photolysis, and the gas phase reaction with hydroxyl radicals, ozone, or nitrate radicals. The most important reaction considered in the hazard assessment of organic compounds is hydrolysis, or the reaction of a chemical substance with water. Because the rate of hydrolysis reactions can change substantially as a function of pH, studies performed in the pH range typically found in the environment (pH 5–9) were considered. The second reaction considered in the assessment is photolysis, the reaction of a chemical with sunlight. Both hydrolysis and photolysis occur in air, water, and soil, while only hydrolysis was considered in sediment. The half-lives for reactive processes, if faster than removal via biodegradation, were used to assign the hazard designation by direct comparison to the DfE persistence criteria.

For the atmospheric compartment, persistence also includes the evaluation of oxidative gas-phase processes. These processes include the reaction with ozone, hydroxyl radicals, and nitrate radicals. Since the average concentration of these oxidative species in the atmosphere has been measured, the experimental or estimated rate constants were converted to, and reported as, a half-life in the assessment using standard pseudo first-order kinetics (U.S. EPA 2011f; U.S. EPA 2011d).

For inorganic compounds, an additional chemical process was considered, the potential to be reduced or oxidized (undergo a redox reaction) under environmental conditions. Redox reactions change the oxidation state of the species through the transfer of electrons to form another compound (such as the reduction of Cr(VI) to Cr(III). A change in the oxidation state of a metal

or inorganic species can result in significant change in the material's hazard designation, in this example going from Cr(VI) to Cr(III) makes the compound less toxic.

Transport

The persistence of a chemical substance is based on determining the importance of removal processes that may occur once a chemical enters the environment. As noted in Section 4.3, chemicals with a half-life of less than 60 days are expected to be at most a Moderate hazard designation for persistence. Persistence does not directly address the pathways in which a chemical substance might enter the environment (e.g., volatilization or disposal in a landfill) and focuses instead on the removal processes that are expected to occur once it is released into air, water, soil, or sediment. Similarly, the persistence assessment does not address what might happen to a chemical substance throughout its life cycle, such as disposal during incineration of consumer or commercial products. Understanding the environmental transport of a chemical substance can help identify processes relevant to environmental assessment. For example, if a chemical is toxic to benthic organisms and partitions primarily to sediment, its potential release to water should be carefully considered in the selection of alternatives.

Biodegradation

In the absence of rapid hydrolysis or other chemical reactions, biodegradation is typically the primary environmental degradation process for organic compounds. Determining the importance of biodegradation is, therefore, an important component of the assessment. Biodegradation processes are divided into two types. The first is primary biodegradation, in which a chemical substance is converted to another substance. The second is ultimate biodegradation, in which a chemical is completely mineralized to small building-block components (e.g., CO_2 and water). DfE persistence criteria use data that are reported as a percent removal in the guideline ready biodegradability test or as a half-life in other experimental studies; both of these measurements can be compared directly to the DfE criteria in 4.1.2. When considering primary degradation, the assessment process includes an evaluation of the potential for the formation of metabolites that were more persistent than the parent materials. Chemical substances that undergo rapid primary degradation but only slow ultimate biodegradation were considered to have stable metabolites. In the absence of measured data on the substance of interest, DfE will evaluate the potential for biodegradation for chemicals with a MW <1,000 daltons using the EPA EPISuite™ models. EPISuite™ estimates the probability for ready biodegradation as well as the potential for primary and ultimate removal, as described in Section 4.3. A default Very High persistence hazard designation was assigned for polymers with a MW >1,000 daltons according to SF Polymer Assessment guidance (U.S. EPA 2010d).

4.4 Evaluating Human Health Endpoints

After data collection and analysis of the physical-chemical properties for the chemicals being assessed the comparison of the data against the hazard criteria can begin. Section. 4.4.1discusses how measured data are used to make hazard designations for human health endpoints and Section 4.2 presents the approach for filling in data gaps to make these hazard designations.

4.4.1 Endpoints Characterized and Evaluated Against Criteria Based on Measured Data

This section provides a short description of how measured data were used to designate the level of hazard for each endpoint. As a reminder, the criteria for the hazard designations are in Table 4-2.

For acute mammalian toxicity the median lethal doses or concentrations were used to assign the hazard designation. Four levels of hazard designation have been defined ranging from Low to Very High.

For cancer the hazard designation was contingent on the level of evidence for increased incidence of cancer, and not potency. The definitions applied in DfE criteria are based on International Agency for Research on Cancer levels of evidence (International Agency for Research on Cancer 2006). For example, a designation of Very High concern requires that the substance be characterized as a "known or presumed human carcinogen", whereas a designation of Low concern requires either negative studies or robust SAR conclusions. A designation of Moderate was applied as a default value when there was an absence of data suggesting High carcinogenicity, and an absence of data supporting Low carcinogenicity (i.e., a lack of negative studies or weak SAR conclusions).

Similarly, the hazard designation for mutagenicity/genotoxicity was also based on the level of evidence rather than potency. Complete data requirements for this endpoint were both gene mutation and chromosomal aberration assays. For instances of incomplete or inadequate mutagenicity/genotoxicity data, a Low hazard designation cannot be given.

For chronic endpoints, such as reproductive, developmental, neurological and repeated dose toxicity, the hazard designation was based on potency. The evaluation considers both lowest observed adverse effect levels (LOAELs) and identification of no observed adverse effect levels (NOAELs) when available. The LOAEL and the NOAEL are experimental dose levels, and their reliability is dictated by the study design. In studies for which the lowest dose tested resulted in an adverse effect (and therefore a NOAEL was not established), and in studies for which the highest dose tested was a NOAEL, a conservative approach using professional judgment was used to address uncertainty regarding the lowest dose or exposure level that might be expected to cause a particular adverse effect. For example, in the absence of an established a NOAEL, an identified LOAEL might fall within the range of a Moderate hazard; however, it is uncertain if a lower dose, such as one that falls within the range of high hazard exists because no lower doses were tested. In such cases, professional judgment was applied to assign a hazard designation when possible. Some degree of uncertainty was evident in results from studies in which a NOAEL may fall within one hazard range (e.g., moderate hazard) and the identified LOAEL falls within a different hazard range (e.g., low hazard) because the true LOAEL may fall in either category, but there were not enough experimental data points to determine the true LOAEL. Professional judgment was also applied to these cases to assign a hazard descriptor when possible and the rationale used was described in the assessment. Developmental neurotoxicity was considered and was evaluated using the developmental toxicity criteria , which are more stringent than the criteria for neurotoxicity, and thus designed to be more protective (U.S. EPA 2011b).

The criteria for skin and respiratory sensitization, which are immune-based responses, consider the frequency and potency of the reactions. For skin sensitization, categories were based on the weight of evidence[11] from traditional animal bioassays, but *in vitro* alternative studies were also considered. At this time, there are no standard test methods for respiratory sensitization; as a result there was often no designation for this endpoint.

The evaluation of skin and eye irritation and corrosivity were based on the time to recovery.

4.4.2 SAR – Application of SAR and Expert Judgment to Endpoint Criteria

If measured data pertaining to human health criteria were not available, potential adverse effects were estimated with SAR analysis. To make these estimates, DfE relied on the expertise of scientists in EPA's New Chemicals Program who have reviewed thousands of chemicals and associated data using these methods. SAR uses the molecular structure of a chemical to infer a physicochemical property that can be related to specific effects on human health. These correlations may be qualitative (simple SAR) or quantitative (QSAR). Information on EPA's use of SAR analysis has been published by U.S. EPA (1994a). Public access to free validated quantitative SAR models for human health endpoints is far more limited than physical-chemical properties, environmental fate parameters, or ecotoxicology.

Carcinogenicity

Carcinogenicity was assessed using the OncoLogic expert system that provides a qualitative result directly applicable to the DfE criteria. For other endpoints that required SAR approaches, an analog approach using expert judgment was used as discussed in Section Table 4-2.

The potential for a chemical to cause cancer in humans was estimated using OncoLogic expert system. This program uses a decision tree based on the known carcinogenicity of chemicals with similar chemical structures, information on mechanisms of action, short-term predictive tests, epidemiological studies, and expert judgment. All estimates obtained in this project were reviewed by EPA scientists having appropriate expertise. Estimates for the other human health endpoints were based on expert judgment using an analog approach and not through the use of computerized SAR methodologies.

Polymers Assessment

Estimates for polymers were typically obtained using the SF Polymer Assessment guidance based on the MW profile (U.S. EPA 2010d). Those polymers with MW >1,000 were assessed using an appropriate representative structure that has a MW less than or equal to the average MW. For polymers with an average MW >1,000 daltons and a significant amount of low MW material <1,000 daltons, the low MW components were also assessed for their environmental

[11] Generally, weight of evidence is defined as the process for characterizing the extent to which the available data support a hypothesis that an agent causes a particular effect U.S. EPA (1999a). Guidelines for Carcinogen Risk Assessment, Review Draft. Office of Research and Development. **CEA-F-0644**, U.S. EPA (2002). A Review of the Reference Dose and Reference Concentration Processes. Risk Assessment Forum. December 2002 Final Report. Washington, DC, EPA. **EPA/630/P-02/002F**, U.S. EPA (2005b). Guidelines for Carcinogen Risk Asessment. Risk Assessment Forum. Washington, DC, EPA. **EPA/630/P-03/001F**.. T

fate and potential toxicity in order to identify any possible hazards for the most bioavailable fraction. Similarly, the presence of unreacted monomers requires that the assessment consider these components for polymers of any MW range. The properties for polymers with an average MW >1,000 with no low MW components were generally evaluated as a single high MW material for each of the properties described below. In general, polymers with an average MW >1,000 were not amenable to the available SAR estimation methods and based on the SF guidance are assumed to have low to no bioavailability. Polymers with MW >1,000 that were not degradable or reactive are also typically not bioavailable. Polymers with an average MW >10,000 have potential for adverse effects due to lung overloading, fibrosis and or cancer. There may be exceptions to the rules of thumb outlined above and as such this guidance should not be held as absolute thresholds.

Polymers and oligomers with MWs <1,000 were assessed using a representative structure for all the MW species anticipated to be present in the mixture. The procedures were essentially identical to those employed for the evaluation of impurities or byproducts in discrete chemicals, although in this case the oligomer with the highest concern was used to drive the hazard designation. Unreacted monomers, if present, were also assessed and considered in the hazard evaluation.

4.5 Evaluating Environmental Toxicity and Fate Endpoints

As with endpoints previously mentioned, the preferred method for the evaluation of environmental endpoints is the use of experimental data. In their absence, the alternatives assessment uses computerized QSAR models developed by EPA for the evaluation of environmental endpoints that can be directly compared to the DfE criteria. When measured data were unavailable, the hazard designation for aquatic toxicity was estimated using EPA's ECOSAR™ software and the persistence designation using models in EPA's EPISuite™ software. As a direct result of the design of these models and their direct application to DfE criteria, the evaluation of environmental endpoints using experimental or estimated data was discussed together in the following subsections.

4.5.1 Aquatic Toxicity

For ecological toxicity, the alternatives assessment focused on the hazard designations for acute and chronic studies on freshwater species of algae, invertebrates, and fish, (often referred to as the 'three surrogate species'). Aquatic toxicity values were reported in the assessment as follows:

- Acute (estimated or experimental) - LC_{50} in mg/L
- Chronic (experimental) - No observed effect concentration (NOEC) in mg/L ; and
- Chronic (estimated) - ChV, or the geometric mean between the NOEC and the LOEC, in mg/L

Experimental data reported in the alternatives assessment also included information on the species tested. Test data on other organisms (e.g., worms) were included in the assessment if data were readily available. These data would be evaluated using professional judgment to support hazard designations assigned using the three surrogate species; however they were not used by themselves to assign a hazard designation as DfE criteria are not available

If an experimental or estimated effect level exceeded the known water solubility of a chemical substance, or if the log K_{ow} exceeded the estimated ECOSAR™ cut-off values for acute and chronic endpoints (which are class specific), NES were predicted for the aquatic toxicity endpoints. NES indicates that at the highest concentration achievable, the limit of a chemical's water solubility, no adverse effects were observed (or would be expected). In these cases, a Low hazard designation was assigned. In the cases where both an estimated water solubility and ECOSAR™ estimate were used, then an additional factor of ten was applied to the water solubility before a NES designation was assigned to account for the combined uncertainty in the model estimates.

In the case where an experimental aquatic toxicity value was significantly higher than the chemical's water solubility, it was likely the result of a poorly conducted study. In this circumstance, which is generally more frequent for formulated products or mixtures, additional details were provided in the data quality section to describe why the reported values could not be used to assign a hazard designation.

EPA's ECOSAR™ estimation program uses chemical structure to estimate toxicity of a chemical substance using class-specific QSARs. ECOSAR™ automatically determines all of the classes that a chemical substance may belong to and, therefore, may provide a number of different ecotoxicity estimates for some or all of the species and durations estimated. Modeled results are dependent on the functional groups present on the molecule as well as the diversity of chemicals with experimental data that were used to build the models. The hazard profiles report every estimated value returned from ECOSAR™. However, the hazard designation was based on the most conservative ECOSAR™ estimate, unless expert judgment suggested that an individual substance was better represented by a specific class based on analysis of the operative mechanism of action. Experimental log K_{ow} values were used preferentially as input into ECOSAR™. In their absence, estimated log K_{ow} values from EPISuite™ were used.

The QSARs for ECOSAR™ were built using experimental data for several chemical classes. For a chemical class to be defined within ECOSAR™, sufficient acute experimental data were required to build a QSAR for all three species included in the model. There were instances, however, where sufficient experimental data are not available to build a chronic QSAR for some of the three surrogate species. When ECOSAR™ did not provide chronic estimates, the acute value (experimental or estimated) was divided by an acute to chronic ratio (ACR) to arrive at the chronic value. ACRs of 10 were used for fish and daphnid and an ACR of 4 was used for algae (Mayo-Bean, Nabholz et al. 2011) .

An estimate of NES is the default value used for organics, oligomers, or non-ionic polymers with a MW >1,000 daltons in the assignment of aquatic toxicity hazard. In EPA's New Chemical program, aquatic toxicity is not predicted for chemicals with a MW >1,000 daltons as uptake has been found to decrease exponentially with MWs >600 daltons (Nabholz, Clements et al. 1993) due to a decrease in passive absorption through respiratory membranes (Mayo-Bean, Nabholz et al. 2011).

4.5.2 Bioaccumulation

Bioaccumulation is a process in which a chemical substance is absorbed in an organism by all routes of exposure as occurs in the natural environment, e.g., from dietary and ambient environment sources. Bioaccumulation is the net result of the competing processes; this includes uptake, metabolism and elimination of a chemical in an organism. Bioaccumulation can be evaluated using the BAF, the steady state ratio of a chemical in an organism relative to its concentration in the ambient environment, where the organism is exposed through ingestion and direct contact. Experimental BAFs have not been widely available in the scientific literature and, as a result, experimental BCFs are more commonly used to evaluate the bioaccumulation hazard. BCFs are defined as the ratio of the concentration of a chemical in an organism to the concentration of the chemical in the organism's surroundings; BCFs are typically measured for fish (in water) using guideline studies.

Experimental BAF or BCF values can be compared directly to the DfE criteria for this endpoint to assign a hazard designation. The BCF/BAF designations range from <100 for a Low designation to >5,000 for a Very High Designation (see 4.1.2). If experimental values were available for both of these endpoints, and the BCF and BAF were >100 (i.e., above the Low designation), the largest factor was used to assign hazard designation. If experimental BCFs <100 were available, the estimated upper trophic BAF from EPISuite™ was used preferentially if its use resulted in a more conservative hazard designation and the potential for metabolism was accurately accounted for within the model estimates.

In the absence of experimental data, evaluation of bioaccumulation potential can be done using the log K_{ow} and the log octanol/air partition coefficient K_{oa} as estimated by EPISuite™. However, analysis using K_{oa} requires the use of metabolism data for higher trophic, air breathing organisms, which can be difficult to obtain from the scientific literature and cannot be readily estimated. BAFs and BCFs from EPISuite™ were, therefore, typically used for the bioaccumulation hazard designation when experimental data were lacking. These values can be compared directly to DfE criteria and the most conservative result was used for the hazard designation. For chemicals that had estimated bioaccumulation data, available experimental monitoring data were used to provide insight into the reliability of the model results. For example, an estimated Low bioaccumulation potential may be increased to a Moderate designation if a chemical was routinely identified in samples from higher trophic levels, or a High designation if the chemical was routinely measured in animals at the top of the food chain.

An estimate of Low is the default value used for discrete organics with a MW >1,000 daltons in the assignment of bioaccumulation hazard. This assignment is consistent with an analysis of the chemicals used in the development the bioconcentration and bioaccumulation estimation programs in the EPISuite™ software (U.S. EPA 2011g). The training sets for these models included 527 and 421 chemicals, respectively, with a MW range 68-992 (959 for BAF) daltons. Given that BCF and BAF reach a maximum and then decrease with increasing log K_{ow}, a default value of Low is in general consistent with the limited bioavailability expected for materials with a MW >1,000 daltons. DfE will use all available well-conducted studies when evaluating bioaccumulation potential for materials with a MW >1,000, including environmental biomonitoring data on higher trophic levels.

For polymers with a MW >1,000 daltons, the default bioaccumulation designation was Low, arising from their limited bioavailability (U.S. EPA 2010d).

4.5.3 Environmental Persistence

A chemical's persistence in the environment is evaluated by determining the type and rate of potential removal processes. These removal processes were generally divided into two categories: chemical and biological. Of the chemical degradation processes, an evaluation of environmental persistence includes the reaction of a chemical with water, also known as hydrolysis, because water is ubiquitous in the environment. Hydrolysis rate constants can be obtained from the literature or estimated, and the resulting half-lives can be compared directly to DfE criteria. For commercial chemicals, hydrolysis tends to be a slower environmental removal process than biodegradation. Direct and indirect photolysis also represent other potential chemical degradation processes that are considered in the alternative assessment, and they are discussed later in this section.

Biodegradation, the most prevalent biological removal processes, were divided into two types. The first is primary biodegradation, in which a chemical substance is converted to another substance through a single transformation. The second is ultimate biodegradation, in which a chemical is completely mineralized to small building-block components (e.g., CO_2 and water). DfE criteria utilize ultimate biodegradation preferentially for the persistence hazard designation, although primary removal rates were informative in assigning hazard designations particularly for materials that were transformed slowly, and to a lesser extent for those that are transformed rapidly.

If ultimate biodegradation data were not available, primary removal data were used in some cases. For primary removal processes, the potential for the formation of degradation products that are more persistent than the parent compounds must be considered in the hazard designation. When present, the persistent degradation products should be evaluated for fate and toxicity. Half-life data on the persistent degradation products, if available, were used to determine the assignment for the persistence designation. In the absence of persistent degradation products, primary biodegradation half-life data were compared directly to the DfE criteria to assign a hazard designation.

Biodegradation processes can be classified as either aerobic or anaerobic. Aerobic biodegradation is an oxidative process that occurs in the presence of oxygen. Anaerobic biodegradation is a reductive process that occurs only in the absence of oxygen. Aerobic biodegradation is typically assessed for soil and water, while anaerobic biodegradation is generally assessed in sediment. For determining the persistence hazard, the importance of both aerobic and anaerobic biodegradation as well as partitioning and transport in the environment were considered to determine what removal processes were most likely to occur.

One aspect of the assessment is to determine the potential for biodegradation of a chemical substance within a sewage treatment plant and other environments. In this assessment, the term "ready biodegradability" refers to a chemical's potential to undergo removal in guideline laboratory studies. A positive result in a test for ready biodegradability can be considered as indicative of rapid and ultimate degradation in most environments including biological sewage

treatment plants. Ready tests typically include a 10-day window, beginning when the biodegradation parameter (e.g., dissolved organic carbon, theoretical oxygen demand) reaches 10%. The 10-day window must occur within the 28-day length of the test. If the pass level of the test (typically 60%) is met in the 10-day window, the chemical received a Very Low hazard designation. Those that did not pass the 10-day window criterion but met the pass level in 28 days, received a Low hazard designation. If ready biodegradability test data were available but the chemical did not meet the pass level, the chemical was evaluated based on measured data using the DfE half-life criteria (Table 4-1). These half-life criteria were also used to assign a hazard designation for non-guideline ultimate biodegradation studies reported in the scientific literature.

In the absence of a reported half-life, experimental data were also used to approximate half-life as appropriate. For example, a chemical that undergoes <5% removal in 30 days would be expected to have a half-life >60 days and would be assigned a High persistence concern.

When experimental data on the biodegradation of a chemical substance were not available, the potential of that substance to undergo this removal process was assessed from the results of the EPISuite™ models. These models fall into one of four classes: Rapid biodegradation models based on linear and non-linear regressions that estimate the probability that a chemical substance will degrade fast; Expert survey models that determine the rate of ultimate and primary biodegradation using semi-quantitative methods; Probability of ready biodegradability; and Probability of rapid biodegradation under anaerobic conditions. Each of these is discussed in the following paragraphs.

The first models (Biowin 5 and 6) used in the screening assessment estimated ready biodegradability (also known as Japanese Ministry of International Trade and Industry (MITI) models), and provided the probability that a material passes this standardized test. Those chemicals that were estimated to pass the ready biodegradability test received a Low persistence designation. If a chemical was not estimated to pass the MITI test, the results of the other EPISuite™ biodegradation models were used.

The rapid biodegradation potential models within EPISuite™ (Biowin 1 and 2) were useful for determining if a chemical substance was expected to biodegrade quickly in the environment. If a chemical was likely to biodegrade quickly, it was generally assigned a Low hazard designation for persistence. The results of the estimates from these models may be used in concert with the semi-quantitative output from a second set of models, which include an ultimate and primary survey models (Biowin 3 and 4) for evaluating persistence. These models provided a numeric result, ranging from 1 to 5, as an indication of the amount of time required for complete mineralization (ultimate degradation) and removal of the parent substance (primary degradation) of the test compound. The numeric result was converted to an estimated half-life for removal that can be compared directly to DfE criteria. If results from different models (other than the MITI models) led to a different hazard designation, then the ultimate biodegradation model results were used preferentially. If the transport properties indicate the potential for the material to partition to sediment, an anoxic compartment, then the results of the anaerobic probability model (Biowin 7) will also be evaluated.

Half-lives for hydrolysis from experimental studies or EPISuite™ estimates were used in preference to biodegradation data when they suggested that hydrolysis is a more rapid removal process. Hydrolysis half-lives were compared directly to DfE criteria to assign the persistence designation. Similar to primary biodegradation, breakdown products resulting from hydrolysis were evaluated for fate and toxicity when they were expected to be more persistent than the parent compound.

Photolysis may also be an important environmental removal process. In general, environmental removal rates from photolysis do not compete with biodegradation or hydrolysis although there are exceptions such as iodides. Photolysis may be an important removal process for chemicals that were not bioavailable because of their limited water solubility. Estimation methods for photolysis rates were not available using computerized SAR tools. If experimental or suitable analog data were available, the rate of photolysis was evaluated relative to other removal processes.

When evaluating the environmental persistence designation, it should be noted that chemicals with a High or Very High designation can degrade over time, although this process may occur at a very slow rate. As a result, a Very High designation may have been assigned if persistent degradates were expected to be produced, even at a very slow rate, in the absence of experimental biodegradation data for the parent substance.
Chemicals that contain a metal were assigned a High persistence designation in the assessment, as these inorganic moieties are recalcitrant. In this instance, an 'R' footnote was added to the hazard summary table to indicate that the persistence potential was based on the presence of a recalcitrant inorganic moiety. The assessment process also included the evaluation of the potential chemical reactions of metal-containing and inorganic moieties to determine if they were potentially transformed to more or less hazardous forms.

Polymers with a MW >1,000 generally received a Very High persistence designation due to their lack of bioavailability.

4.6 Endocrine Activity

Chemicals included in DfE alternatives assessments were screened for potential endocrine activity, consistent with the DfE Alternatives Assessment Criteria. Chemicals included in DfE alternatives assessments were screened for potential endocrine activity, consistent with the DfE Alternatives Assessment Criteria. **Endocrine activity** refers to a change in endocrine homeostasis caused by a chemical or other stressor. An **endocrine disruptor** is an external agent that interferes in some way with the role of natural hormones in the body, in a manner causing adverse effects. Relevant data were summarized in the hazard assessments for each chemical, located in Section 4.8. Data on endocrine activity were available for decaBDE and some of the alternatives included in this report. For chemicals without available data on endocrine activity, this was acknowledged with a "no data located" statement. When endocrine activity data were available, the data were summarized as a narrative. A unique hazard designation of Low, Moderate or High was not provided in Table 4-2, for reasons discussed below.

The document *Special Report on Environmental Endocrine Disruption: An Effects Assessment and Analysis* describes EPA's activities regarding the evaluation of endocrine disruption (U.S.

EPA 1997). This report was requested by the Science Policy Council and prepared by EPA's Risk Assessment Forum. This report states that "Based on the current state of the science, the Agency does not consider endocrine disruption to be an adverse endpoint per se, but rather to be a mode or mechanism of action potentially leading to other outcomes, for example, carcinogenic, reproductive or developmental effects, routinely considered in reaching regulatory decisions" (U.S. EPA 1997). The report also states that "Evidence of endocrine disruption alone can influence priority setting for further testing and the assessment of results of this testing could lead to regulatory action if adverse effects are shown to occur" (U.S. EPA 1997).

The 1996 Food Quality Protection Act directed EPA to develop a scientifically-validated screening program to determine whether certain substances may cause hormonal effects in humans. In response, EPA established the Endocrine Disruptor Screening Program (EDSP) (U.S. EPA 2012b). The EDSP is developing requirements for the screening and testing of thousands of chemicals for their potential to affect the endocrine system. When complete, EPA will use these screening and testing approaches to set priorities and conduct further testing when warranted. The science related to measuring and demonstrating endocrine disruption is relatively new, and validated testing methods at EPA are still being developed.

The EDSP uses a two-tiered approach that includes initial screening followed by more in-depth testing when warranted (U.S. EPA 2011a). The Tier 1 screening battery is intended to identify chemicals with the potential to interact with the estrogen, androgen, or thyroid hormone systems through any of several recognized modes of action. Positive findings for Tier 1 tests screen for potential for an interaction with endocrine systems, but do not fully characterize the nature of possible effects in whole animals. Tier 2 testing is intended to confirm, characterize, and quantify the effects for chemicals that interact with estrogen, androgen, and thyroid hormone systems. These test methods must undergo a four-stage validation process (protocol development, optimization/prevalidation, validation, and peer-review) prior to regulatory acceptance and implementation. This validation is ongoing for Tier 1 and Tier 2 methods[12]. . Once validated test methods have been established for screening and testing of potential endocrine disruptors, guidance must be developed for interpretation of these test results using an overall weight-of-evidence characterization.

To assess the data on endocrine activity, DfE applies the weight of evidence approach developed by the EDSP (U.S. EPA 2011c). This process integrates and evaluates data, and always relies on professional judgment (U.S. EPA 2011c). To evaluate endocrine activity with this weight of evidence approach, DfE examined multiple lines of evidence (when available) and considered the nature of the effects within and across studies, including number, type, and severity/magnitude of effects, conditions under which effects occurred (e.g., dose, route, duration), consistency, pattern, range, and interrelationships of effects observed within and among studies, species, strains, and sexes, strengths and limitations of the *in vitro* and *in vivo* information, and biological plausibility of the potential for an interaction with the endocrine, androgen, or thyroid hormonal pathways.

Most test data for chemicals in this report consist of *in vitro* assays, but results of *in vitro* assays

[12] Information on the status of assay development and validation efforts for each assay in EPA's EDSP can be found at: http://www.epa.gov/oscpmont/oscpendo/pubs/assayvalidation/status.htm

alone were not generally expected to provide a sufficient basis to support a hazard designation for endocrine disruption. EPA expects that *in vivo* evidence would typically be given greater overall influence in the weight of evidence evaluation than *in vitro* findings because of the inherent limitations of such assays. Although *in vitro* assays can provide insight into the mode of action, they have limited ability to account for normal metabolic activation and clearance of the compound, as well as normal intact physiological conditions (e.g., the ability of an animal to compensate for endocrine alterations).

As described in the DfE Alternatives Assessment Criteria, endocrine activity was summarized in a narrative, rather than by High, Moderate or Low hazard designation. The endocrine activity summaries can be found in the hazard profiles. This is an appropriate approach because there is no consensus on what constitutes high, moderate or low concern for this endpoint. The summary of endocrine activity largely relies on representative studies and expert review summaries.

4.7 Hazard Summary Table

Table 4-4 Screening Level Hazard Summary for DecaBDE and Brominated Flame Retardant Alternatives

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from predictive models and/or professional judgment.

[§] Based on analogy to experimental data for a structurally similar compound.

Chemical (for relevant trade names see the synonym section of the individual profiles in Section 4.8)	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
DecaBDE and Brominated Flame Retardant Alternatives (BFRs)																
DecaBDE and Discrete BFR Alternatives																
Bis(hexachlorocyclopentadieno) Cyclooctane	13560-89-9	L	*M*[§]	*M*[§]	VL	VL	L	M	L		VL	*L*	*L*	*L*	VH	*H*
Decabromodiphenyl Ethane	84852-53-9	L	*M*[§]	L	L	VL	*H*[§]	L	L		VL	VL	L	*L*	VH	*H*
Decabromodiphenyl Ether	1163-19-5	L	M	L	L	H	H	M	L		L	L	*L*	*L*	VH	*H*
Ethylene Bis-tetrabromophthalimide	32588-76-4	L	*M*[§]	L	*L*	L	*M*[§]	L	*L*		VL	VL	*L*	*L*	VH	*H*
Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether	21850-44-2	L	*M*	M	*M*	*M*	*L*	*M*	*M*		*L*	*L*	*L*	*L*	VH	*H*
Tris(tribromoneopentyl) Phosphate	19186-97-1	*L*	*M*	*M*	*L*	*H*	*H*	*M*	*H*		*L*	*L*	*L*	*L*	*H*	*M*
Tris(tribromophenoxy) Triazine	25713-60-4	L	*L*	L	*L*	*L*	*L*	L	L		L	VL	*L*	*L*	VH	*H*

Table 4-4 Continued

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from predictive models and/or professional judgment.

[d] This hazard designation is driven by potential for lung overloading as a result of dust forming operations.

♦ Different formulations of the commercial product are available. One of these many formulations has an average MW of ~1,600 and contains significant amounts of lower MW components. These lower MW components are primarily unchanged starting materials that have hazard potentials different than the polymeric flame retardant, as follows: VERY HIGH- Estimated potential for bioaccumulation; HIGH-Experimental concern for acute aquatic toxicity; HIGH-Estimated potential for chronic aquatic toxicity; MODERATE-Experimental concern for developmental; and MODERATE-Estimated potential for carcinogencity, genotoxicity, repeated dose, reproductive, and skin and respiratory sensitization toxicity

¤ This alternative may contain impurities. These impurities have hazard designations that differ from the flame retardant alternative, Confidential Brominated Polymer, as follows, based on experimental data: HIGH for human health, HIGH for aquatic toxicity, VERY HIGH for bioaccumulation, and VERY HIGH for persistence

T This chemical is subject to testing in an EPA consent order.

Chemical (for relevant trade names see the synonym section of the individual profiles in Section 4.8)	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Brominated Flame Retardants (BFRs) Continued																
Polymeric BFRs																
Brominated Epoxy Resin End-Capped with Tribromophenol	135229-48-0	*L*	*L*	L	*L*	*L*	*L*	*M*[d]	L		L	VL	*L*	*L*	*VH*	*L*
Brominated Polyacrylate	59447-57-3	*L*	*L*	*L*	*L*	*L*	*L*	*M*[d]	*L*		*L*	*L*	*L*	*L*	*VH*	*L*
Brominated Polystyrene	88497-56-7	L	*L*	*L*	*L*	*L*	*L*	*M*[d]	*L*		L	*L*	*L*	*L*	*VH*	*L*
Confidential Brominated Epoxy Polymer #1	Confidential	*L*	*L*	*L*	*L*	*L*	*L*	*M*[d]	*L*		*L*	*L*	*L*	*L*	*VH*	*L*
Confidential Brominated Epoxy Polymer #2	Confidential	*L*	*L*♦	*L*♦	*L*♦	*L*♦	*L*	*M*♦[d]	*L*♦	♦	*L*	*L*	*L*♦	*L*♦	*VH*	*L*♦
Confidential Brominated Epoxy Polymer Mixture #1	Confidential	*L*	*L*♦	*L*♦	*L*♦	*L*♦	*L*	*M*♦[d]	*L*♦	♦	*L*	*L*	*L*♦	*L*♦	*VH*	*L*♦
Confidential Brominated Epoxy Polymer Mixture #2	Confidential	*L*	*L*♦	*L*♦	*L*♦	*L*♦	*L*	*M*♦[d]	*L*♦	♦	*L*	*L*	*L*♦	*L*♦	*VH*	*L*♦
Confidential Brominated Polymer	Confidential	*L*	*L*¤	L	*L*¤	*L*¤	*L*¤	*L*¤	*L*	*L*	L	VL	*L*	*M*[T]¤	VH [T]	*M*[T]¤
TBBPA Glycidyl Ether, TBBPA Polymer	68928-70-1	*L*	*L*♦	*L*♦	*L*♦	*L*♦	*L*	*M*♦[d]	*L*♦	♦	*L*	*L*	*L*♦	*L*♦	*VH*	*L*♦

Table 4-5 Screening Level Hazard Summary for Organic Phosphorus Nitrogen Flame Retardant Alternatives

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from predictive models and/or professional judgment.

[d] This hazard designation is driven by potential for lung overloading as a result of dust forming operations. [§] Based on analogy to experimental data for a structurally similar compound. [‡] The highest hazard designation of any of the oligomers with MW <1,000. [◊] The highest hazard designation of a representative component of the oligomeric mixture with MWs <1,000. [¥] Phosphonate Oligomer, with a MW range of 1,000 to 5,000, may contain significant amounts of an impurity, depending on the final product preparation. This impurity has hazard designations that differ from the polymeric flame retardant, as follows: MODERATE-Experimental concern for repeated dose, skin sensitization and eye irritation; and HIGH-Experimental concern for reproductive, developmental, acute aquatic toxicity.

Chemical (for relevant trade names see the synonym section of the individual profiles in Section 4.8)	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Organic Phosphorus or Nitrogen Flame Retardants (PFRs or NFRs) Alternatives																
Discrete PFR, NFR and P/NFR Alternatives																
Substituted Amine Phosphate Mixture [1]	Confidential	*H*	*M*	*M*	*M*	*M*	*L*	*M*	*M*	*M*[§]	*M*[§]	*VH*	*M*	*L*	*H*	*L*
Triphenyl Phosphate	115-86-6	L	*M*	L	L	L	L	M	L		L	VL	VH	VH	L	M
Polymeric PFR and NFR Alternatives																
Bisphenol A bis-(diphenyl phosphate), BAPP	181028-79-5	L	*L*	L	*L*	*L*[§]	L	L	L		L	L	L	L	H	*H*[◊]
Melamine Cyanurate[1]	37640-57-6	*L*	*M*	*M*	*M*[§]	*M*[§]	*L*	H	*L*		*L*	*L*	*L*	*L*	VH	*L*
Melamine Polyphosphate[1]	15541-60-3	L	*M*	*M*	*L*[§]	*L*	*L*[§]	*M*	L		L	VL	L	L	*H*	*L*
N-alkoxy Hindered Amine Reaction Products	191680-81-6	L	*M*	L	*H*	*H*	*L*	*H*	L		L	VL	*H*	*H*	H	*H*[‡]
Phosphonate Oligomer	68664-06-2	L	*M*	*L*[§]	*L*[¥]	*L*[¥]	*M*[‡¥]	*L*[§¥]	*L*[§¥]		*M*[‡¥]	*M*[‡]	L[¥]	*H*[‡]	*VH*	*H*[‡]
Polyphosphonate	68664-06-2	L	*L*	*L*	*L*	*L*	*L*	*M*[d]	*L*		*L*	*L*	*L*	*L*	*VH*	*L*
Poly[phosphonate-co-carbonate]	77226-90-5	L	*L*	*L*	*L*	*L*	*L*	*M*[d]	*L*		*L*	*L*	*L*	*L*	*VH*	*L*
Resorcinol bis-diphenylphosphate	125997-21-9	L	*M*[§]	L	L	VL	*M*[§]	M	*L*		L	VL	VH	*H*[‡]	M	*H*[‡]

[1] Hazard designations are based upon the component of the salt with the highest hazard designation, including the corresponding free acid or base.

Table 4-6 Screening Level Hazard Summary for Inorganic Flame Retardant Alternatives

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from predictive models and/or professional judgment.

[d] This hazard designation is driven by potential for lung overloading as a result of dust forming operations.

[R] Recalcitrant: Substance is comprised of metallic species that will not degrade, but may change oxidation state or undergo complexation processes under environmental conditions.

* Ongoing studies may result in a change in this endpoint

Chemical (for relevant trade names see the synonym section of the individual profiles in Section 4.8)	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Inorganic Flame Retardant Alternatives																
Aluminum Diethylphosphinate	225789-38-8	L	*L*	L	*L*	*M*	*M*	L	L		L	VL	M	M	H^R	*L*
Aluminum Hydroxide	21645-51-2	L	*L*	L	*L*	L	M	L	L		VL	VL	*M*	*M*	H^R	*L*
Ammonium Polyphosphate	68333-79-9	L	*L*	*L*	*L*	*L*	*L*	*M*[d]	L		VL	L	*L*	*L*	*VH*	*L*
Antimony Trioxide[1]	1309-64-4	L	L*	L	*L*	*L*	*L*	M*	L		L	M	M	M	H^R	*L*
Magnesium Hydroxide	1309-42-8	L	L	L	*L*	*L*	*L*	L	*L*		M	*M*	*L*	*L*	H^R	*L*
Red Phosphorus	7723-14-0	VH	*L*	*M*	*L*	*L*	*L*	*L*	L		M	H	L	L	H	*L*
Zinc Borate	1332-07-6	L	*L*	*H*	*M*	*M*	*H*	*L*	L		L	L	*H*	*H*	H^R	*L*

[1] This compound is included in the ongoing EPA Work Plan evaluation for Antimony and Compounds

4.8 Hazard Evaluations

Aluminum Diethylphosphinate

Screening Level Hazard Summary

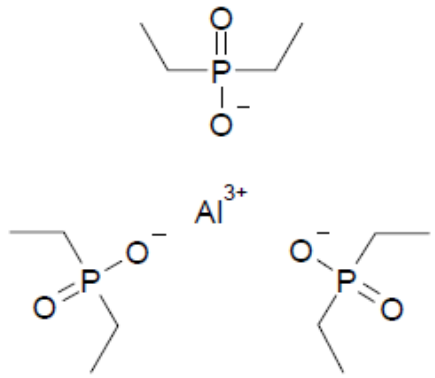
This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

[R] Recalcitrant: Substance is comprised of metallic species that will not degrade, but may change oxidation state or undergo complexation processes under environmental conditions

		Human Health Effects											Aquatic Toxicity		Environmental Fate	
Chemical	CASRN	Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Aluminum Diethylphosphinate	225789-38-8	L	*L*	L	*L*	*M*	*M*	L	L		L	VL	M	M	*H* [R]	*L*

Aluminum Diethylphosphinate

<table>
<tr><td colspan="2">  </td><td>CASRN: 225789-38-8</td></tr>
<tr><td colspan="2"></td><td>MW: 390.27</td></tr>
<tr><td colspan="2"></td><td>MF: 3 $C_4H_{11}PO_2 \cdot Al$</td></tr>
<tr><td colspan="2"></td><td>Physical Forms:
Neat: Solid</td></tr>
<tr><td colspan="2"></td><td>Use: Flame retardant</td></tr>
<tr><td colspan="3">SMILES: CCP(=O)(CC)O[Al](OP(=O)(CC)CC)OP(=O)(CC)CC</td></tr>
<tr><td colspan="3">Synonyms: Exolit OP 930, Aluminium diethylphosphinate, Aluminium tris(diethylphosphinate)</td></tr>
<tr><td colspan="3">Chemical Considerations: This alternative is an inorganic compound and in the absence of experimental data professional judgment using chemical class and structural considerations were used to complete this hazard profile.</td></tr>
<tr><td colspan="3">Polymeric: No
Oligomers: Not applicable</td></tr>
<tr><td colspan="3">Metabolites, Degradates and Transformation Products: None</td></tr>
<tr><td colspan="2">Analog: Confidential aluminum metal salts
Endpoint(s) using analog values: Absorption, distribution, metabolism & excretion, carcinogenicity, reproductive and developmental effects, immunotoxicity, neurotoxicity</td><td>Analog Structure: Not applicable</td></tr>
<tr><td colspan="3">Structural Alerts: Not applicable</td></tr>
<tr><td colspan="3">Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).</td></tr>
<tr><td colspan="3">Hazard and Risk Assessments: DfE Alternatives Assessment for Flame Retardants in Printed Circuit Boards, Review Draft, November 8, 2008.</td></tr>
<tr><td colspan="3">U.S. EPA TSCA Regulatory Status: This chemical is not listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.</td></tr>
</table>

Aluminum Diethylphosphinate CASRN 225789-38-8			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	Decomposes at 315 (Measured)	Submitted confidential study	Adequate.
	Decomposes at 300 (Measured)	Submitted confidential study	
	Decomposes at 330 (Measured)	De Boysère and Dietz, 2005	Sufficient details were not available to assess the quality of this study.
	Decomposes at >300 (Measured)	Clariant, 2007	Sufficient details were not available to assess the quality of this study.
	>400 (Measured)	NICNAS, 2005	Sufficient details were not available to assess the quality of this study.
Boiling Point (°C)	Expected to decompose before boiling (Estimated)	Professional judgment	Based on available data for melting point.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2011	Cutoff value for compounds that are anticipated to be nonvolatile, according to SF assessment guidance.
Water Solubility (mg/L)	2.5×10^{3} (Measured)	Submitted confidential study	Sufficient details were not available to assess the quality of this study. Aluminum diethylphosphinate has low wettability and very slow dissolution. This gives a kinetically controlled solubility of <1 mg/L by guideline 92/69/EEC A.6. If aluminum diethylphosphinate is formed by precipitation of a soluble salt, the remaining equilibrium solubility of 2.5×10^{3} mg/L is found. This can be assumed to be the true limit of solubility under ideal conditions.

Aluminum Diethylphosphinate CASRN 225789-38-8			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	<1 (Measured) According to guideline 92/69/EEC A.6	NICNAS, 2005; Submitted confidential study	Guideline study; aluminum diethylphosphinate has low wettability and very slow dissolution. If aluminum diethylphosphinate is formed by precipitation of a soluble salt, the remaining equilibrium solubility of 2.5×10^{3} mg/L is found, which can be assumed to be the true limit of solubility under ideal conditions.
Log K_{ow}	-0.44 (Estimated)	Stuer-Lauridsen et al., 2007; Beard and Marzi, 2005	Reported in a secondary source; it is unclear whether this value reflects the chemical's low water solubility or its lipophobicity.
Flammability (Flash Point)	Not readily combustible according to guideline 96/69/EEC, test A.10. (Measured)	Submitted confidential study	Guideline study.
	No self-ignition below 402°C (Measured)	Submitted confidential study	Adequate.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Pyrolysis	Major products are diethylphosphinic acid, ethylphosphonic acid, phosphoric acid, and their respective salts (Measured)	Beard and Marzi, 2005	Study details and test conditions were not available.
pH	4.0 (Measured)	Beard and Marzi, 2005	Value was reported in conference presentation authored by Clariant Corp. and UMSICHT. Value suggests the potential for dissolution.

Aluminum Diethylphosphinate CASRN 225789-38-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
pK_a		Dissociated within 24 hours at pH 4.5 during MITI test (Measured)	NICNAS, 2005	Available data suggest that this compound is likely to dissociate under environmental conditions. However, it has potential for dissociation as a function of pH that will have a significant influence on its environmental fate. Available data are not adequate to assess its dissociation under typical environmental conditions.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Based on estimates of physical and chemical properties, analogs, and professional judgment, aluminum diethylphosphinate is determined to not be readily absorbed through skin but is absorbed through the inhalation of dust and oral exposure.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	Absorption as neat solid negligible through skin. Absorption good through lungs. Absorption good through gastrointestinal tract. (Estimated)	Professional judgment	Estimates based on physical/chemical properties and confidential analogs.
Acute Mammalian Toxicity		**LOW: Experimental studies indicate that oral and dermal routes to rats do not produce substantial mortality at levels up to 2,000 mg/kg. There were no lethality data located for inhalation exposure.**		
Acute Lethality	**Oral**	Rat oral LD_{50} >2,000 mg/kg	NICNAS, 2005	Reported in a secondary source. Test substance was Exolit OP 930.
	Dermal	Rat dermal LD_{50} >2,000 mg/kg	NICNAS, 2005	Reported in a secondary source. Test substance was Exolit OP 930.
	Inhalation			No data located.
Carcinogenicity		**LOW: Aluminum diethylphosphinate is estimated to be of low hazard for carcinogenicity based on comparison to analogous metal salts and professional judgment.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)	Not expected to be carcinogenic (Estimated)	Professional judgment	Estimated based on analogy to confidential metal salts.

Aluminum Diethylphosphinate CASRN 225789-38-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Combined Chronic Toxicity/ Carcinogenicity			No data located.
Genotoxicity		**LOW: Experimental studies indicate that aluminum diethylphosphinate does not cause gene mutations in bacteria or chromosomal aberrations in mammalian cells.**		
	Gene Mutation *in vitro*	Negative, Ames Assay	NICNAS, 2005	Reported in a secondary source.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	Negative, chromosomal aberrations in CHL cells	NICNAS, 2005	Reported in a secondary source.
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: Aluminum diethylphosphinate is estimated to be of low hazard for reproductive effects resulting from the presence of a bioavailable metal species, by professional judgment based on a comparison to analogous metal salts.**		
	Reproduction/ Developmental Toxicity Screen	Expected to have low hazard potential for reproductive effects (Estimated)	Professional judgment	Estimated based on analogy to confidential metal salts.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Reproduction and Fertility Effects			No data located.

Aluminum Diethylphosphinate CASRN 225789-38-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**MODERATE: Aluminum diethylphosphinate is estimated to be of moderate hazard for developmental effects resulting from the presence of a bioavailable metal species, by professional judgment based on a comparison to analogous metal salts.**		
	Reproduction/ Developmental Toxicity Screen	Expected to have a moderate hazard potential for developmental effects resulting from the presence of bioavailable metal species. (Estimated)	Professional judgment	Estimated based on analogy to confidential metal salts.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Prenatal Development			No data located.
	Postnatal Development			No data located.
Neurotoxicity		**MODERATE: Aluminum diethylphosphinate is estimated to be of moderate hazard for neurotoxicity, due to the presence of a bioavailable metal species, based on comparison to analogous metal salts and professional judgment.**		
	Neurotoxicity Screening Battery (Adult)	Expected to have a moderate hazard potential for neurotoxic effects resulting from the presence of bioavailable metal species. (Estimated)	Professional judgment	Estimated based on analogy to confidential metal salts.
		Rat NOAEL >1,000 mg/kg	Beard and Marzi, 2005	Study details and test conditions were not available.
Repeated Dose Effects		**LOW: Experimental studies indicate that oral exposure to rats produces no adverse effects at levels up to 1,000 mg/kg/day.**		
		28- day NOAEL >1,000 mg/kg/day, rats	NICNAS, 2005	Reported in a secondary source. Test substance was Exolit OP 930.
Skin Sensitization		**LOW: Negative for skin sensitization in guinea pigs.**		
	Skin Sensitization	Non-sensitizing, guinea pigs	NICNAS, 2005	Reported in a secondary source.
Respiratory Sensitization		**No data located.**		
	Respiratory Irritation			No data located.

Aluminum Diethylphosphinate CASRN 225789-38-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Eye Irritation		**LOW: Aluminum diethyphosphinate is slightly- to non-irritating in rabbit eyes.**		
	Eye Irritation	Slightly irritating, rabbits	NICNAS, 2005	Reported in a secondary source.
		Not irritating, rabbits (Confidential)	Submitted confidential study	Study reported in a submitted confidential study.
Dermal Irritation		**VERY LOW: Aluminum diethylphosphinate is not irritating to rabbit skin.**		
	Dermal Irritation	Non-irritating, rabbit	NICNAS, 2005	Reported in a secondary source.
Endocrine Activity		**No data located.**		
				No data located
Immunotoxicity		**Aluminum diethylphosphinate is estimated to be of moderate hazard for immunotoxicity, due to the presence of a bioavailable metal species, based on comparison to analogous metal salts and professional judgment.**		
	Immune System Effects	Expected to have a moderate hazard potential for immunotoxicity effects resulting from the presence of bioavailable metal species. (Estimated)	Professional judgment	Estimated based on analogy to confidential metal salts.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**MODERATE: The measured green algae EC_{50} is between 10 and 100 mg/L. For fish and *Daphnia*, adequate toxicity values have not been determined; reported values are not LC_{50} but the highest dose tested.**		
Fish LC_{50}		Zebra fish 96-hour LC_{50} >11 mg/L (Experimental)	NICNAS, 2005	Reported in a secondary source.
		Zebra fish 96-hour LC_{50} >9.2 mg/L (Experimental, Confidential)	Submitted confidential study	Study reported in a submitted confidential study.
Daphnid LC_{50}		*Daphnia magna* 48-hour LC_{50} >33.7 mg/L (Experimental)	NICNAS, 2005	Reported in a secondary source.
		Daphnia magna 48-hour LC_{50} >33 mg/L (Experimental, Confidential)	Submitted confidential study	Study reported in a submitted confidential study.
Green Algae EC_{50}		*Scenedesmus subspicatus* 72-hour E_bC_{50} of 60 mg/L (Experimental); *Scenedesmus subspicatus* 72-hour E_rC_{50} of 76 mg/L (Experimental)	NICNAS, 2005	Reported in a secondary source.

Aluminum Diethylphosphinate CASRN 225789-38-8			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	72-hour EC_{50} = 50mg/L (Experimental, Confidential)	Submitted confidential study	Study reported in a submitted confidential study.
Chronic Aquatic Toxicity	**MODERATE: Experimental values for green algae are between 1 mg/L and 10 mg/L, while measured toxicity values for fish and *Daphnia* are >10 mg/L.**		
Fish ChV	48 mg/L (Estimated, Confidential)	Submitted confidential study	Study reported in a submitted confidential study.
Daphnid ChV	*Daphnia magna* 21-day EC_{50} = 22.3 mg/L for immobility (Experimental) *Daphnia magna* 21-day EC_{50} = 46.2 mg/L for reproduction (Experimental) *Daphnia magna* 21-day LOEC = 32 mg/L for immobility and reproduction (Experimental) *Daphnia magna* 21-day NOEC = 10 mg/L for immobility and reproduction (Experimental)	NICNAS, 2005	Reported in a secondary source.
Green Algae ChV	1.8 mg/L (Experimental, Confidential)	Submitted confidential study	Study reported in a submitted confidential study.

Aluminum Diethylphosphinate CASRN 225789-38-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**Although the behavior of metal salts under environmental conditions is dependent on the characteristics of the local environment (predominately pH), transport of both the metal species and the organic anion is anticipated to be dominated by leaching through soil, runoff to aqueous environments, adsorption and/or precipitation of the metal ion onto soil or sediment, and wet and dry deposition dust particulates in air to land or surface water. Volatilization of this ionic compound from either wet or dry surfaces is not expected to be an important fate process. Nevertheless, the environmental fate of this organic salt will be dependent on its pH-dependent dissociation, and adequate data are not available.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment	Cutoff value for nonvolatile compounds.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}			No data located.
	Level III Fugacity Model			This substance is not amenable to the model.

Aluminum Diethylphosphinate CASRN 225789-38-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Persistence		**VERY HIGH: For the organic counter-ion, estimates indicate that the half-life for ultimate aerobic biodegradation in water is less than 60 days, which converts to moderate potential for persistence. However, the metal ion is recalcitrant to biodegradation or other typical environmental removal processes.**		
Water	**Aerobic Biodegradation**	**Organic counter-ion:** Days-weeks (primary survey model) Weeks (ultimate survey model)	EPI	
		Metal ion: Recalcitrant (Estimated)	Professional judgment	Metal ions will not degrade in the environment.
		Not inherently biodegradable (Measured)	Stuer-Lauridsen et al., 2007	Sufficient details were not available to assess the quality of this study.
		Not readily biodegradable (Measured)	NICNAS, 2005	Reported in a secondary source.
		Not readily biodegradable (Measured)	Stuer-Lauridsen et al., 2007	Sufficient details were not available to assess the quality of this study.
	Volatilization Half-life for Model River	Not a significant fate process (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	Not a significant fate process (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
Soil	**Aerobic Biodegradation**	Respiration inhibition of activated sludge microorganisms LC_{50} = 1968 mg/L, NOEC = 483 mg/L. (Measured)	NICNAS, 2005; Submitted confidential study	Reported in a secondary source.
	Anaerobic Biodegradation	No degradation (Measured)	Stuer-Lauridsen et al., 2007	Sufficient details were not available to assess the quality of this study.
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	Not a significant fate process (Estimated)	Professional judgment	This chemical is expected to exist entirely in particulate form in air.

Aluminum Diethylphosphinate CASRN 225789-38-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
	Hydrolysis	Metal salts form a variety of hydroxylation products as a function of pH. Hydrolysis of the organic counter-ion is not expected to be a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The organic counter ion does not contain functional groups that would be expected to hydrolyze readily under environmental conditions.
Environmental Half-life		**Organic counter-ion**: <60 days **Metal ion**: Recalcitrant (Estimated)	EPI; Professional judgment	Based on estimated biodegradation half-lives for the organic counter-ion and metal ions will not degrade in the environment.
Bioaccumulation		**LOW: Aluminum diethylphosphinate is not expected to have potential for bioaccumulation.**		
	Fish BCF	<100 (Estimated)	Professional judgment	Available data suggests this chemical will dissociate under environmental conditions.
	BAF			No data located.
	Metabolism in fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

Beard, A; Marzi, T. New phosphorus based flame retardants for E&E applications: A case study on their environmental profile in view of European legislation on chemicals and end-of-life (REACH), WEEE, RoHS). In *Addcon 2005*, September 20-21, 2005, Hamburg, Germany. **2005.** http://www.flameretardants-online.com/images/userdata/pdf/175_EN.pdf

Boethling, R.S.; Mackay, D. *Handbook of property estimation methods for chemicals: Environmental and health sciences;* Lewis Publishers: Boca Raton, FL, **2000.**

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[SF Assessment Guidance] EPA (Environmental Protection Agency). Sustainable Futures Summary Assessment. *Assessment of Discrete Organic Chemicals.* U.S. Environmental Protection Agency: Washington D.C. **2011**. http://www.epa.gov/oppt/sf/pubs/iad_discretes_092011.pdf

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Aluminum Hydroxide

Screening Level Hazard Summary

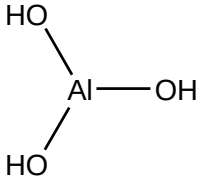
This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

[R] Recalcitrant: Substance is comprised of metallic species that will not degrade, but may change oxidation state or undergo complexation processes under environmental conditions

		Human Health Effects										Aquatic Toxicity		Environmental Fate	
Chemical	CASRN	Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Aluminum Hydroxide	21645-51-2	L	*L*	L	*L*	L	M	L	L		VL	VL	*M*	*M*	*H*[R]	*L*

Aluminum Hydroxide

<table>
<tr><td colspan="2">  </td><td>CASRN: 21645-51-2</td></tr>
<tr><td colspan="2"></td><td>MW: 78.01</td></tr>
<tr><td colspan="2"></td><td>MF: AlH_3O_3</td></tr>
<tr><td colspan="2"></td><td>Physical Forms:
Neat: Solid</td></tr>
<tr><td colspan="2"></td><td>Use: Flame retardant</td></tr>
<tr><td colspan="3">SMILES: O[Al](O)O</td></tr>
<tr><td colspan="3">Synonyms: Aluminum hydroxide ($Al(OH)_3$) (TSCA Inventory); Aluminum trioxide, Gibbsite, Bayersite, Nordstrandite, Aluminum trihydrate</td></tr>
<tr><td colspan="3">Chemical Considerations: This alternative is an inorganic compound and in the absence of experimental data professional judgment using chemical class and structural considerations were used to complete this hazard profile.</td></tr>
<tr><td colspan="3">Polymeric: No
Oligomers: Not applicable</td></tr>
<tr><td colspan="3">Metabolites, Degradates and Transformation Products: None</td></tr>
<tr><td colspan="2">Analog: unspecified analogous aluminum compounds were discussed in the structural based professional judgment rationale.
Endpoint(s) using analog values: carcinogenicity, reproductive effects, immunotoxicity</td><td>Analog Structure: Not applicable</td></tr>
<tr><td colspan="3">Structural Alerts: Aluminum compounds (U.S. EPA, 2010).</td></tr>
<tr><td colspan="3">Risk Phrases: Not classified by Annex I Directive 67/548/EEC & IUCLID (Pakalin, 2007).</td></tr>
<tr><td colspan="3">Hazard and Risk Assessments: Risk assessment completed for aluminum hydroxide by the National Research Council Subcommittee on Flame-Retardant Chemicals (NRC, 2000). Hazard assessment completed for DfE Alternatives Assessment for Flame Retardants in Printed Circuit Boards, Review Draft, November 8, 2008.</td></tr>
<tr><td colspan="3">U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.</td></tr>
</table>

Aluminum Hydroxide CASRN 21645-51-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	Decomposes at approximately 200 (Measured)	European Commission, 2000	Adequate.
	Decomposes at approximately 150-220 to Al_2O_3 and H_2O (Measured)	European Commission, 2000	
	Decomposes (loses water) at 300 (Measured)	Lewis, 2000	
Boiling Point (°C)	The substance is expected to decompose before boiling. (Estimated)	Professional judgment	Based on the values included in the melting point section of this assessment.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2011	Cutoff value for compounds that are anticipated to be nonvolatile, according to SF assessment guidance.
Water Solubility (mg/L)	1.5 at 20˚C (Measured)	European Commission, 2000	Measured values were not consistently reported, but are sufficient for subsequent components of the hazard assessment.
	$1.5x10^{-2}$ at 20 ˚C (Measured)	European Commission, 2000	
	Insoluble in water (Estimated)	Lide, 2006	
	Practically insoluble in water (Estimated)	O'Neil, 2001; Lewis, 2000	
	≤0.09 at 20˚C, pH 6-7 According to OECD 105 flask method (Measured)	ECHA, 2010	Guideline study reporting non-specific value that is in agreement with other experimental values indicating insolubility.
Log K_{ow}			No data located. This inorganic compound is not amenable to available estimation methods.
Flammability (Flash Point)	Not flammable (Estimated)	European Commission, 2000	Adequate.
Explosivity	Not explosive (Estimated)	European Commission, 2000	Adequate.
Pyrolysis			No data located.
pH	pH of a saturated solution in water was 6 to 7 (Measured)	ECHA, 2010	Determined in a water solubility study.

Aluminum Hydroxide CASRN 21645-51-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
pK_a		Not applicable (Estimated)	Professional judgment	Determination of dissociation constant is not possible due to the insolubility of the test substance.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Toxicokinetic data suggest that aluminum hydroxide is not readily absorbed in humans following oral exposure. Excretion occurs primarily through feces, and less so in urine. Animal studies indicated that aluminum accumulated in intestinal cells but was not found in other tissues.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	26Al labeled aluminum hydroxide (in water suspension) was administered to rats by oral gavage. The mean fractional uptake of 26 Al from aluminum hydroxide was 0.025±0.041% Compared to rats injected with 0.19 ng 26Al labeled aluminum citrate in solution, aluminum hydroxide as an insoluble compound is less bioavailable than soluble compounds (mean fractional uptake of 26Al 0.079 ±0.041% 0.0057%).	ECHA 2012	Reported in a secondary source. Adequate, performed in accordance with OECD guidelines and GLP; Aluminium hydroxide, was suspended in water with added 1% carboxymethylcellulose (to maintain a suspension).
		After rats were exposed to aluminum hydroxide in drinking water for 10 weeks, aluminum accumulated in intestinal cells but not in other tissues.	HSDB, 2006	Reported in a secondary source, study details and test conditions were not provided.
		In metabolic studies in humans, 12% of an oral load of aluminum hydroxide was retained, but absorption was not calculated.	HSDB, 2006	Reported in a secondary source, study details and test conditions were not provided.
		The absorbed fraction of aluminum hydroxide in two human males dosed orally was 0.01%.	HSDB, 2006	Reported in a secondary source, study details and test conditions were not provided.

Aluminum Hydroxide CASRN 21645-51-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Adult humans with renal failure who ingested 1.5–3.0 g aluminum hydroxide per day for 20-32 days absorbed between 100 and 568 mg aluminum per day (7-19% of the dose).	HSDB, 2006	Reported in a secondary source, study details and test conditions were not provided.
		Adult humans taking aluminum antacids had a 3-fold increase of aluminum levels in the urine; minimal aluminum was absorbed and was mostly excreted in the feces.	ATSDR, 2008	Reported in a secondary source, study details were not provided.
Acute Mammalian Toxicity		**LOW: Aluminum hydroxide has low acute toxicity based on oral LD_{50} > 2,000 mg/kg-bw in rats.**		
Acute Lethality	**Oral**	Rat oral LD_{50} >5,000 mg/kg bw.	European Commission, 2000	Reported in a secondary source, study details and test conditions were not provided.
		Rat oral LD_{50} > 2,000 mg/kg bw	ECHA, 2012	Reported in a secondary source. Performed in accordance with OECD guidelines and GLP
	Dermal			No data located.
	Inhalation			No data located.
Carcinogenicity		**LOW: Aluminum hydroxide is estimated to be of low hazard for carcinogenicity based on professional judgment and comparison to analogous aluminum compounds.**		
	OncoLogic Results **Carcinogenicity (Rat and Mouse)** **Combined Chronic Toxicity/ Carcinogenicity**	Low potential for carcinogenicity. (Estimated)	Professional judgment	Estimated based on professional judgment and comparison to analogous aluminum compounds.
Genotoxicity		**LOW: Aluminum hydroxide did not cause mutations in bacteria *in vitro* and did not cause chromosomal aberrations *in vitro*.**		
	Gene Mutation *in vitro*	Negative in mouse lymphoma cells with and without metabolic activation	ECHA, 2010	Adequate, performed in accordance with OECD guidelines and GLP.

Aluminum Hydroxide CASRN 21645-51-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*			No data located.
	Chromosomal Aberrations *in vivo*	Negative for induction of micronuclei in polychromatic erythrocytes of bone marrow in Sprague-Dawley rats	ECHA 2010	Adequate, performed in accordance with OECD guidelines and GLP
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: Aluminum hydroxide is estimated to be of low hazard for reproductive effects based on professional judgment and comparison to analogous aluminum compounds.**		
	Reproduction/ Developmental Toxicity Screen	Low potential for reproductive effects. (Estimated)	Professional judgment	Estimated based on professional judgment and comparison to analogous aluminum compounds.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			
Developmental Effects		**LOW: Aluminum hydroxide does not show developmental toxicity when administered orally to rats or mice at dose levels up to 266 mg/kg/day.**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.

Aluminum Hydroxide CASRN 21645-51-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Prenatal Development	Mouse, oral, no developmental effects, NOAEL = 266 mg/kg/day (Highest dose tested)	Domingo et al., 1989	Adequate.
		Mouse, oral, NOAEL = 268 mg/kg/day (Highest dose tested)	Gomez et al., 1989	Abstract only.
		Mouse, oral, NOAEL = 300 mg/kg/day (Only dose tested)	Colomina et al., 1994	Abstract only.
		Rat, oral, NOAEL = 768 mg/kg/day (Highest dose tested)	Gomez et al., 1990	Abstract only.
		Rat, oral, NOAEL = 384 mg/kg/day (Only dose tested)	Llobet et al., 1990	Abstract only.
	Postnatal Development			No data located.
Neurotoxicity		**MODERATE: Aluminum hydroxide is expected to be of moderate hazard for neurotoxicity based on available experimental data.**		
	Neurotoxicity Screening Battery (Adult)	30-day Rat, oral diet, no significant effects noted, NOAEL = 1,252 mg Al/kg/day	ATSDR, 2006	Reported in a secondary source.
		90-day Rat, oral gavage, impaired learning in a labyrinth maze test, LOAEL = 35 mg Al/kg/day as aluminum hydroxide with citric acid	ATSDR, 2006	Reported in a secondary source.
Repeated Dose Effects		**LOW: Aluminum hydroxide is of low hazard for repeated dose effects based on an experimental study indicating no adverse effects in rats following oral doses up to 14,470 ppm (302 mg/kg-day). In addition, a low potential for repeated dose effect is estimated based on professional judgment and comparison to analogous aluminum compounds.**		
		Low potential for repeated dose effects. (Estimated)	Professional judgment	Estimated based on professional judgment and comparison to analogous aluminum compounds.
		28-day Rat (male), oral diet, no systemic effects noted. NOAEL = 14,470 ppm/diet (302 mg aluminum/kg/day)	Hicks et al., 1987	Study details from primary source.

Aluminum Hydroxide CASRN 21645-51-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Skin Sensitization		**LOW: Aluminum hydroxide is not a skin sensitizer.**		
	Skin Sensitization	Low potential for skin sensitization. (Estimated)	Professional judgment	Estimated based on professional judgment and comparison to analogous aluminum compounds.
		Not sensitizing to guinea pigs in an *in vivo* maximization test	ECHA 2012	Reported in a secondary source; conducted in accordance with OECD guidelines and GLP
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**VERY LOW: Aluminum hydroxide is not an eye irritant.**		
	Eye Irritation	Not irritating, rabbits.	ECHA 2012	Reported in a secondary source; Conducted in accordance with OECD guidelines and GLP
Dermal Irritation		**VERY LOW: Aluminum hydroxide is not irritating to skin.**		
Dermal Irritation		Not irritating, rabbits.	ECHA 2012	Reported in a secondary source. Conducted in accordance with OECD guidelines and GLP
		Not irritating, rabbits, mice and pigs	ECHA 2012	Reported in a secondary source; non-guideline studies
Endocrine Activity		**No data located.**		
				No data located.
Immunotoxicity		**Aluminum hydroxide is estimated have potential for immunotoxicity based on professional judgment and comparison to analogous aluminum compounds.**		
	Immune System Effects	Moderate potential for immunotoxicity. (Estimated)	Professional judgment	Estimated based on professional judgment and comparison to analogous aluminum compounds.
		6-Week human, oral, LOAEL = 25 mg Al/kg/day (Reduction in primed cytotoxic T-cells, only dose tested).	ATSDR, 2006	Reported in a secondary source. The toxicological significance of the finding is unknown.
ECOTOXICITY				
ECOSAR Class		Not applicable		

Aluminum Hydroxide CASRN 21645-51-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Acute Toxicity	**MODERATE: Aluminum hydroxide is estimated to be of moderate hazard for acute toxicity based on potential for dissolved aluminum species to cause adverse effects in aquatic species, as described in the EPA New Chemical Categories document which includes inorganic salts of aluminum (Professional judgment).**		
Fish LC_{50}	*Salmo trutta* 96-hour NOEC >100 mg/L (Experimental)	European Commission, 2000	Reported in a secondary source. The effect concentration is greater than the measured water solubility.
Daphnid LC_{50}	*Daphnia magna* 48-hour NOEC >100 mg/L (Experimental)	European Commission, 2000	Reported in a secondary source. Study details and test conditions were not available and the effect concentration is greater than the measured water solubility.
	Daphnia magna 48-hour NOEC > 0.135 mg/L (measured)	ECHA, 2012	Study conducted with aluminum powder
	Daphnia magna 48-hr EC_{50} = 0.8240 mg/L (Measured)	TSCATS, 1996	Study incorrectly cited in source; results are for a different test substance, vanadium hydroxide oxide.
Green Algae EC_{50}	*Selenastrum capricornutum* 72-hour NOEC >100 mg/L (Experimental)	European Commission, 2000	Reported in a secondary source. The effect concentration is greater than the measured water solubility.
	Selenastrum capricornutum 96-hr EC_{50} = 0.6560 mg/L (Measured)	TSCATS, 1996	Study incorrectly cited in source; results are for a different test substance. vanadium hydroxide oxide.
	Pseudokirchnerella subcapitata 96-hr EC_{50} = 0.46 mg/L (measured)	ECHA, 2012	Reported in a secondary source. EC_{50} range: 0.57 mg/L at pH of 7.6 and 0.46 mg/L at pH of 8.2. The water solubilities of aluminum hydroxide under basic pHs are not available; experimental details are not sufficient to address the confidence limits of these data points.
	Pseudokirchnerella subcapitata 72-hour NOEC = 0.004 – 0.052 mg/L	ECHA, 2012	Reported in a secondary source. DfE criteria is based on LC and EC_{50} values; therefore a NOEC value is not sufficient to determine a hazard designation.

Aluminum Hydroxide CASRN 21645-51-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Chronic Aquatic Toxicity		**MODERATE: Aluminum hydroxide is estimated to be of moderate hazard for chronic aquatic toxicity based on potential for dissolved aluminum species to cause adverse effects in aquatic species, as described in the EPA Chemical Categories document which includes inorganic salts of aluminum (Professional judgment).**		
Fish ChV		*Pimephales promelas* 42-da NOEC = 0.102 mg/L, LOEC = 0.209 mg/L (Measured)	TSCATS, 1996	Study incorrectly cited in source; results are for a different test substance, vanadium hydroxide oxide.
Daphnid ChV		*Daphnia magna* 21-da NOEC = 0.091 mg/L, LOEC = 0.197 mg/L (Measured)	TSCATS, 1996	Study incorrectly cited in source; results are for a different test substance, vanadium hydroxide oxide.
Green Algae ChV				No data located.
ENVIRONMENTAL FATE				
Transport		**Although the behavior of aluminum salts under environmental conditions is dependent on the characteristics of the local environment (predominately pH), transport of the aluminum (III) species is anticipated to be dominated by leaching through soil; runoff to aqueous environments; adsorption and/or precipitation of the metal ion onto soil or sediment; and wet and dry deposition dust particulates in air to land or surface water. Volatilization of this ionic compound from either wet or dry surfaces is not expected to be an important fate process. Under acidic pHs typically encountered in the environment, it may form insoluble polymeric aluminum hydroxide colloids while under basic conditions, anionic aluminum hydroxide is expected to predominate. Other factors influencing its behavior include the presence of dissolved organic matter, the extend of absorbtion on suspended particles, and the presence of other aluminum species.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment	Cutoff value for non-volatile compounds.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; EPA, 2011	Cutoff value for non mobile compounds according to SF assessment guidance.
	Level III Fugacity Model			No data located.
Persistence		**HIGH: As an inorganic material, aluminum hydroxide is not expected to biodegrade or oxidize, under typical environmental conditions. Aluminum hydroxide does not absorb light at environmentally relevant wavelengths and is not expected to photolyze. No degradation processes for aluminum hydroxide under typical environmental conditions were identified.**		

Aluminum Hydroxide CASRN 21645-51-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment	Substance is or contains inorganic elements, such as metal ions or oxides, that are expected to be found in the environment >180 days after release.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law constant.
Soil	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment	Substance contains inorganic elements.
	Anaerobic Biodegradation	Recalcitrant (Estimated)	Professional judgment	Substance contains inorganic elements.
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	>1 year (Estimated)	Professional judgment	Substance contains inorganic elements.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Professional judgment	Aluminum hydroxide does not absorb UV light at environmentally relevant wavelengths and is not expected to undergo photolysis.
	Hydrolysis			Dissociation of aluminum hydroxide in environmental waters is dependent both on the pH and the local concentration of other aluminum species; dissociation will not occur unless in highly acidic waters, e.g., pH 3.
Environmental Half-Life				No data located. Inorganic compounds are outside the estimation domain (EPI).
Bioaccumulation		**LOW: Aluminum hydroxide is not expected to bioaccumulate.**		

Aluminum Hydroxide CASRN 21645-51-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Fish BCF	<100 (Estimated)	Professional judgment	Aluminum hydroxide is an inorganic compound and is not anticipated to bioaccumulate or bioconcentrate. This inorganic compound is not amenable to available (Q)SAR models.
	BAF	<100 (Estimated)	Professional judgment	
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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[SF Assessment Guidance] EPA (Environmental Protection Agency). Sustainable Futures Summary Assessment. *Assessment of Discrete Organic Chemicals*. U.S. Environmental Protection Agency: Washington D.C. **2011**. http://www.epa.gov/oppt/sf/pubs/iad_discretes_092011.pdf

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Ammonium Polyphosphate

Screening Level Hazard Summary

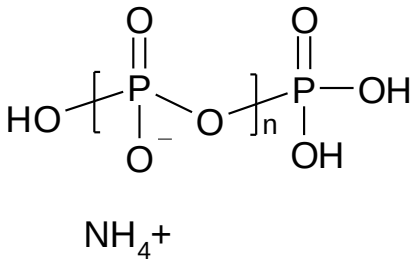
This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

[d] This hazard designation is driven by potential for lung overloading as a result of dust forming operations.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Ammonium Polyphosphate	68333-79-9	L	*L*	*L*	*L*	*L*	*L*	*M*[d]	L		VL	L	*L*	*L*	*VH*	*L*

Ammonium Polyphosphate



CASRN: 68333-79-9

MW: ~100,000

MF: $(NH_4)_k \cdot H_{(n+2-k)}P_nO_{(3n+1)}$ (NAS, 2000)

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: This polymer inorganic salt with MW >1,000 and no low MW components is not amenable to SMILES notation.

Synonyms: Polyphosphoric acids, ammonium salts (TSCA Inventory); AP 422, AP 462, APP (fireproofing agent), APP 422, Albaplas AP 95, Amgard CL, Amgard MC, Amgard TR, Ammonium polyphosphate, Ammonium polyphosphates, Antiblaze MC, Antiblaze MCM, Budit 3076, Budit 3076DC, Budit 3077, Budit 365, DFP-I, EINECS 269- 789-9, Exolit 462, Exolit 263, Exolit 422, Exolit 442, Exolit 454, Exolit 455, Exolit 462, Exolit 470, Exolit AP 422, Exolit AP 423, Exolit AP 462, FR-Cros 480, FR-Cros 484,Fire-Trol LCG-R, Flameguard PT 8, Hostaflam 423, Hostaflam AP 420, Hostaflam AP 422, Hostaflam AP 462, Hostaflam AP 464, Hostaflam TP-AP 751, Hostaflam TP-AP 752, Novawhite, Phos-Chek P 30, Phos-Chek P 40, Phos-Chek P 60, Poly-N 10-34-0, Poly-N 11-37-0, Polymetaphosphoric acid, ammonium salt, Polyphosphoric acid, ammonium salt, Sumisafe, Taien A, Taien H

Chemical Considerations: High-molecular ammonium polyphosphate (n>50) with a minimum of water-soluble fractions are being used to an increasing extent in flame retardants (Gard, 2005, Schrödter et al., 2005). These insoluble ammonium polyphosphates are long chain, ionic phosphate polymers with the following molecular formula: $(NH_4)_k \cdot H_{(n+2-k)}P_nO_{(3n+1)}$, where n typically can range from 70 (Wanjie International Co., 2007) to >1,000 (Pinfa, 2010). MWs can be as high as 100,000 g/mole and oligomers with a MW <1,000 are not expected. The high MW inorganic polymer was assessed as a non-bioavailable material. Prior assessments for similar polyphosphates evaluated the lower, water soluble moieties, which also have application as a flame retardant.

Polymeric: Yes
Oligomers: Not applicable

Metabolites, Degradates and Transformation Products: Ammonia

Analog: No analogs
Endpoint(s) using analog values: Not applicable

Analog Structure: Not applicable

Structural Alerts: Not applicable

Risk Phrases: Not classified by Annex I Directive 67/548/EEC & IUCLID (Pakalin et al., 2007)

Hazard and Risk Assessments: The Maine Department of Environmental Protection (MDEP) Safer Alternative Assessment for Decabromodiphenyl Ether Flame Retardant in Plastic Pallets includes a Green Screen Assessment of Ammonium Polyphosphate (MDEP, 2007) although these were performed on lower MW materials.

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.

Ammonium Polyphosphate CASRN 68333-79-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)			No data located.
Boiling Point (°C)	>250, decomposition with evolution of ammonia and phosphoric acid (Measured)	Clariant, 1999	Reported in chemical datasheet, consistent with the high melting point expected for this chemical.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large high MW polymers according to SF polymer assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large high MW polymers according to SF polymer assessment guidance.
	0.5 % (w/w) at 25ºC (Measured in 10% suspension)	Clariant, 2009	Inadequate. This value likely represents a dispersion and is not an indication of the material's true water solubility.
	0.5-0.05% max. at 25ºC (Measured in 10% suspension)	Wanjie International Co., 2007	Inadequate. This value likely represents a dispersion and is not an indication of the material's true water solubility.
Log K_{ow}			No data located; polymers with a MW >1,000 are outside the domain of the available estimation methods.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	5.5-7.5 (Measured) At 25ºC in 10% suspension	Clariant, 1999	Measured by chemical supplier. Data are likely for the formulated material in water, and would be dependent on the ammonium/polyphosphate ratios.
pK_a			No data located.

Ammonium Polyphosphate CASRN 68333-79-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Absorption is not expected for any route of exposure. This inorganic polymer moiety is large with a MW >1,000. Based on professional judgment, it is expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No absorption is expected for all routes of exposure if insoluble in water (Estimated)	Professional judgment	Estimated based on physical/chemical properties and limited bioavailability.
Acute Mammalian Toxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is of low potential for acute mammalian toxicity. This low hazard designation is also supported by a rat oral median lethal dose (LD_{50}) of >2,000 mg/kg, a rat dermal LD_{50} of >2,000 mg/kg, and a 4-hour rat median lethal concentration (LC_{50}) of >5.09 mg/L.**		
Acute Lethality	**Oral**	Rat oral LD_{50} >2,000 mg/kg	UNEP, 2008	Although limited study details were reported in a secondary source, results indicated that LD_{50} values were greater than the high dosages tested.
		Rat oral LD_{50} = 4,740 mg/kg	IUCLID, 2000; Clariant, 2009	Although limited study details were reported in a secondary source, results indicated that LD_{50} values were greater than the high dosages tested; data for commercial mixture Exolit 422 (purity not specified).
		Rabbit oral LD_{50} >2,000 mg/kg	UNEP, 2008	Although limited study details were reported in a secondary source, results indicated that LD_{50} values were greater than the high dosages tested.
	Dermal	Rat dermal LD_{50} >5,000 mg/kg	IUCLID, 2000; UNEP, 2008	Although limited study details were reported in a secondary source, results indicated that LD_{50} values were greater than the high dosages tested; data for commercial mixture Exolit 456 (90% ammonium polyphosphate and 10% monoammonium phosphate).

Ammonium Polyphosphate CASRN 68333-79-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Rat dermal LD_{50} >2,000 mg/kg	UNEP, 2008	Although limited study details were reported in a secondary source, results indicated that LD_{50} values were greater than the high dosages tested.
	Inhalation	Rat Inhalation 4-hour LC_{50} >5.09 mg/L	UNEP, 2008	Although limited study details were reported in a secondary source, results indicate that LC_{50} values are greater than the highest concentration tested; it is unspecified if the inhaled substance is a vapor/gas or dust/mist/fume.
Carcinogenicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have few to no residual monomers. Additionally, crosslinking, swellability, dispersability, reactive functional groups, inhalation potential, and hindered amine groups are not expected. Therefore, there is low potential for carcinogenicity based on professional judgment and the SF polymer assessment guidance. No data located.**		
	OncoLogic Results **Carcinogenicity (Rat and Mouse)** **Combined Chronic Toxicity/ Carcinogenicity**	Limited bioavailability expected; crosslinking swellability, dispersability, reactive functional groups, inhalation potential, and hindered amine groups are not expected. (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
Genotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for genotoxicity.**		
	Gene Mutation *in vitro*	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
		Negative, Ames assay, *Salmonella Typhimurium* TA98. TA100, TA1535, TA1537, TA1538, and *E. coli* WP2uvrA; with and without metabolic activation	ESIS, 2000	Reported in a secondary source, study details and test conditions were not provided.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*			No data located.

Ammonium Polyphosphate CASRN 68333-79-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for reproductive effects based on professional judgment and the SF polymer assessment guidance. No data located.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			
Developmental Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for developmental effects based on professional judgment and SF polymer assessment guidance. No data located.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			
	Postnatal Development			

Ammonium Polyphosphate CASRN 68333-79-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Neurotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for neurotoxicity based on professional judgment and the SF polymer assessment guidance. No data located.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
Repeated Dose Effects		**MODERATE: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability; however, because the number average molecular weight (MW_n is >10,000, there is the possibility of lung overloading in dust forming conditions if the compound is insoluble in water. Based on professional judgment and the SF polymer assessment guidance. No data located.**		
		Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
		This polymer MW_n is >10,000; There is uncertain potential for lung effects from lung overload if respirable particles are inhaled; Polymers with a MW >10,000 have the potential for irreversible lung damage as a result of lung overloading. (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
Skin Sensitization		**LOW: Not a skin sensitizer in guinea pigs.**		
	Skin Sensitization	Not a skin sensitizer, guinea pigs	Safepharm, 1993	Reported in chemical data sheet; adequate study details provided.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**VERY LOW: Mixtures containing primarily ammonium polyphosphate were not irritating to rabbit eyes.**		
	Eye Irritation	Not irritating, rabbits	UNEP, 2008	Reported in secondary source; study details and test conditions were not provided; data for commercial mixture (70% ammonium polyphosphate and 30% monoammonium phosphate).

Ammonium Polyphosphate CASRN 68333-79-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Not irritating, rabbits	ESIS, 2000	Reported in a secondary source; study details and test conditions were not provided; data for commercial mixture Exolit 456 (90% ammonium polyphosphate and 10% monoammonium phosphate). Study in accordance with OECD 405 guideline.
Dermal Irritation		**LOW: Mixtures containing primarily ammonium polyphosphate were not irritating to slightly irritating to skin of rabbits.**		
	Dermal Irritation	Not irritating, rabbits 4-hour occlusion	UNEP, 2008	Reported in a secondary source; study details and test conditions were not provided; data for commercial mixture (70% ammonium polyphosphate and 30% monoammonium phosphate).
		Slightly irritating, rabbits; 24-hour occlusive patch test	ESIS, 2000; IUCLID, 2000	Reported in a secondary source; study details and test conditions were not provided; data for commercial mixture Exolit 422 (purity not specified).
		Not irritating	ESIS, 2000; IUCLID, 2000	Reported in a secondary source; study details and test conditions were not provided; data for commercial mixture Exolit 456 (90% ammonium polyphosphate and 10% monoammonium phosphate). Study in accordance with OECD 404 guideline.
Endocrine Activity		**This polymer is large, with a MW >1,000. It is not expected to have endocrine activity due to its poor bioavailability and inability to be readily metabolized in the body based on professional judgment.**		
		Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.

Ammonium Polyphosphate CASRN 68333-79-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Immunotoxicity		**This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for immunotoxicity based on professional judgment and the SF polymer assessment guidance. No data located.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**LOW: Water insoluble polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to have no effects at saturation (NES). These polymers have NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Based on professional judgment, guidance for the assessment of aquatic toxicity hazard leads to a low concern for those materials that display NES. Experimental data are also consistent with this hazard designation.**		
Fish LC_{50}		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
		Oncorhynchus mykiss 96-hour LC_{50} >101 mg/L (experimental)	IUCLID, 2000; UNEP, 2008	Inadequate; limited study details reported in a secondary source and value is much greater than the anticipated water solubility.
		Danio rerio 96-hour LC_{50} = 100 – 1,000 mg/L (experimental)	Clariant, 2009	Inadequate; limited study details reported in a secondary source and value is much greater than the anticipated water solubility.
		Brachydanio rerio 96-hour LC_{50} >500 mg/L (experimental)	IUCLID, 2000	Guideline study red in a secondary source with limited study details; OECD 203. Test substance: Exolit 456 (90% ammonium polyphosphate and 10% of ammonium phosphate).

Ammonium Polyphosphate CASRN 68333-79-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Daphnid LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity	**LOW: Water insoluble polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to have NES. These polymers have NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Based on professional judgment, guidance for the assessment of aquatic toxicity hazard leads to a low potential for those materials that display NES.**		
Fish ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.

Ammonium Polyphosphate CASRN 68333-79-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that this ionic polymer is anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of $<10^{-8}$ atm-$m^{3/}$mole indicates that it is not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that it is not anticipated to migrate from soil into groundwater and also has the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large high MW polymers according to SF polymer assessment guidance.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to adsorb strongly to soil and sediment according to SF polymer assessment guidance.
	Level III Fugacity Model			This substance is not amenable to the model.
Persistence		**HIGH: This polymer is large, with a MW >1,000. It is expected to have negligible water solubility and poor bioavailability to microorganisms indicating that biodegradation is not expected to be an important removal process in the environment. Hydrolysis is expected for ammonium polyphosphates, mainly via end-clipping of a monophosphate unit to form monoammonium phosphate. Hydrolysis rates increase with increasing chain lengths, but reach a limit when n>50. Qualitative statements from manufacturers indicate hydrolysis is slow, but increases with prolonged exposure to water and elevated temperatures. Therefore, hydrolysis is not expected to occur at a rate that would greatly reduce the polymeric chain. Furthermore, long-chain ammonium polyphosphates produced for flame retardant applications may be formulated with melamine or other stabilizers that impede hydrolysis. The polymer does not contain functional groups that would be expected to absorb light at environmentally-relevant wavelengths. Evaluation of these degradation values suggest a half-life for the polymer is >180 days.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large high MW polymers according to SF polymer assessment guidance.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.

Ammonium Polyphosphate CASRN 68333-79-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation	Recalcitrant (Estimated)	Professional judgment	The substance has a MW >1,000 and is not anticipated to be assimilated by microbial populations; therefore, biodegradation is not expected.
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	Not a significant fate process (Estimated)	Professional judgment	This substance is expected to exist entirely in particulate form in air and is not anticipated to undergo gas-phase chemical reactions.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.

Ammonium Polyphosphate CASRN 68333-79-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Hydrolysis	Not a significant fate process (Estimated)	Gard, 2005; Wanjie International Co., 2007; Pinfa, 2010; EFRA, 2011; Professional judgment	Hydrolysis is expected, mainly via end-clipping of a monophosphate unit to form monoammonium phosphate. Qualitative statements from manufacturers indicate hydrolysis is slow, but increases with prolonged exposure to water and elevated temperatures. Hydrolysis is not expected to occur at a rate that would greatly reduce the polymeric chain to a MW <1,000 g/mole.
Environmental Half-life		>180 days (Estimated)	Professional judgment	The substance has a MW >1,000 and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to be removed by other degradative processes under environmental conditions because of limited water solubility and limited partitioning to air.

Ammonium Polyphosphate CASRN 68333-79-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Bioaccumulation		**LOW: This ionic polymer is large, with a MW >1,000. It is expected to have negligible water solubility and poor bioavailability indicating that it will have low potential for bioaccumulation based on professional judgment.**		
	Fish BCF	<100 (Estimated)	Professional judgment	The substance has a MW >1,000 and is not anticipated to be assimilated by aquatic organisms; therefore, bioconcentration is not expected.
	BAF			No data located.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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Antimony Trioxide

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

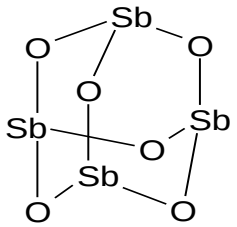
§ Based on analogy to experimental data for a structurally similar compound.

[R] Recalcitrant: Substance is comprised of metallic species that will not degrade, but may change oxidation state or undergo complexation processes under environmental conditions

* Ongoing studies may result in a change in this endpoint

Chemical	CASRN	Human Health Effects										Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitizer	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Antimony Trioxide	1309-64-4	L	L*	L	*L*	*L*	*L*	M*	L		L	M	M	M	*H*[R]	*L*

Antimony Trioxide



Representative Structure

CASRN: 1309-64-4

MW: 291.5

MF: Sb_2O_3 (Empirical)

Physical Forms:
Neat: Solid

Use: Flame retardant synergist

SMILES: O=[Sb]O[Sb]=O (Empirical)

Synonyms: Antimony oxide (TSCA Inventory); Antimony white; Antimony (III) oxide; Antimonious oxide; Antimony sesquioxide; C.I. Pigment White 11; Diantimony trioxide; Patox C; Thermoguard B; Timonox; Timonox White Star; Flowers of antimony; Exitelite; Senarmonite; Valentinite; Weiss-piessglanz

Chemical Considerations: This alternative is an inorganic compound. In the absence of experimental data, professional judgment using chemical class and structural considerations were used to complete this hazard profile.

Polymeric: No
Oligomers: Not applicable

Metabolites, Degradates and Transformation Products: None

Analog: Confidential antimony-containing salts and compounds
Endpoint(s) using analog values: Chronic aquatic toxicity; reproductive and neurological toxicity

Analog Structure: The analogs are confidential and cannot be suitably represented here.

Structural Alerts: None

Risk Phrases: R40: Limited evidence of a carcinogenic effect (EU RAR, 2008) and H351 – suspected of causing cancer by inhalation (ESIS, 2012)

Hazard and Risk Assessments: Risk assessment completed for antimony trioxide by the European Union in 2008 (EU RAR, 2008) and the Subcommittee on Flame-Retardant Chemicals (NRC, 2000).

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.

Antimony Trioxide CASRN 1309-64-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	656 (Measured)	ICSC, 2005	Adequate; measured in the absence of oxygen.
	655 (Measured)	OECD SIAP, 2008	
	655 for the mineral valentinite 570 for the mineral senarmontite (Measured)	Lide, 2008	
Boiling Point (°C)	1,425 (Measured)	ICSC, 2005; Lide, 2008; O'Neil, 2011	Adequate; decomposes on heating.
	1,550 (Measured)	ATSDR, 1992; ICSC, 2005; OECD SIAP, 2008	Reported as sublimation temperature.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2011	Cutoff value for compounds that are anticipated to be nonvolatile, according to SF assessment guidance.
	1 mm Hg at 574°C (Measured)	Sax, 1979; EU RAR, 2008	Value measured at a nonstandard temperature. Result consistent with a vapor pressure below criteria cutoffs.
Water Solubility (mg/L)	14 at 30°C (Measured)	ICSC, 2005	Water solubility of antimony trioxide is pH dependent; pH for this measurement not provided.
	20 at pH 5; 30 at pH 9 (Measured)	Umwelt Bundes Amt, 2001	Reported values, which span a relatively narrow range, are consistently reported in secondary sources.
	19.7 at pH 5; 25.6 at pH 7; 28.7 at pH 9 Ten grams of the Sb_2O_3 was mixed with 100 mL distilled water; agitated for 24 hours at 20°C, filtered an analyzed using atomic absorption. (Measured)	EU RAR, 2008	

Antimony Trioxide CASRN 1309-64-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	2.76 at pH 8 100 mg Sb_2O_3 in 1-L reconstituted water after 7 days (Measured)	Canada, 2010; OECD SIAP, 2008	This value, reported in secondary sources with limited details, is one order of magnitude (10 times) less than other reported values listed above. The difference between these values (approximately 3 and 30 mg) has no impact on the other endpoints in this assessment and may be a result of a typographical error in either study, differences in study methods, analysis, or reporting.
	<28.7 (Measured)	ERMA, 2011	Sufficient details were not available to assess the quality of this study.
	Dissolution in water decreases from pH 1 to pH 7. Above pH 7, the solubility increases rapidly to pH 8, at which point a new equilibrium is established. (Measured)	OECD SIAP, 2008	Within multiple studies the data demonstrate the pH dependency of antimony trioxide solubility.
Log K_{ow}			No data located; inorganic compounds are outside the estimation domain of EPI.
Flammability (Flash Point)	Not combustible (Measured)	ICSC, 2005	Adequate.
Explosivity	Not expected (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Pyrolysis	Not applicable (Estimated)	Professional judgment	Inorganic compounds do not undergo pyrolysis.
pH		Professional judgment	This substance is not expected to produce ions that would alter the pH of the solution in aqueous conditions.

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
pK_a				Not applicable; inorganic compounds are outside the estimation domain of SPARC.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Antimony trioxide is expected to have no absorption through skin and has poor absorption through the lungs and gastrointestinal (GI) tract according to experimental data. Following oral exposure, the majority of antimony trioxide is excreted in the feces. The compound accumulates in lungs with inhalation exposure due to slow absorption and clearance.**		
Dermal Absorption *in vitro*		A percutaneous study in human skin showed 0.26% absorption.	OECD SIAP, 2008	Reported in a secondary source, limited study details provided.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal, or Inhaled**	Not absorbed through the skin; poor absorption through the lung and GI tract (Estimated by analogy)	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/chemical properties.
		Absorption in rats orally administered 2% antimony trioxide in the diet was distributed to the thyroid, GI contents, spleen, heart, bone, muscle, lungs, liver, and GI tissue. The highest concentrations (concentrations not specified) were found in the whole blood, thyroid, and bones. The majority (99%) is excreted in the feces and also in urine within 7 days post-exposure.	NTP, 2005; OECD SIAP, 2008	Reported in a secondary source, limited study details provided.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Six groups of Sprague-Dawley rats were administered antimony trioxide i.p., i.v., or by gavage (100 or 1,000 mg/kg-bw). Following oral administration, antimony trioxide had low absorption (0.3% of 100 mg/kg-bw; 0.05% of 1,000 mg/kg-bw), with a C_{max} at 24 hours and slower elimination from the blood. Antimony underwent significant distribution to the tissues with the majority being found in bone marrow and thyroid, followed by the ovaries, spleen, liver, lung, heart, femur, and skin. The majority of antimony trioxide was excreted in the feces and also in urine.	ECHA, 2011	Reported in a secondary source.
		Occupationally exposed smelter workers had increased (unspecified) levels of antimony in blood and urine following inhalation exposure	NTP, 2005	Reported in a secondary source, occupational reports, no exposure or duration details; detected concentrations not specified.
		Antimony has been detected in low (unspecified) amounts in human breast milk, placenta, amniotic fluid, umbilical cord blood, and fetal liver.	OECD SIAP, 2008	Reported in a secondary source, limited study details provided. Detected concentrations not specified.
	Dermal			No data located.
	Inhalation	Occupational studies measured elevated antimony levels in the lungs of smelter workers both deceased and still living (retired ~20 years) indicating that antimony accumulates and is retained in the lungs long after exposure stopped; measured antimony in the lungs of deceased smelter workers were 12 times greater than unexposed referents	IRIS, 2002; NTP, 2005	Reported in a secondary source, limited study details provided. Detected concentrations not specified.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Fischer 344 rats (65/sex/group) were exposed (whole-body) to antimony trioxide dust at target concentrations of 0, 0.05, 0.5, or 5.0 mg/m^3 (duration-adjusted concentrations: 0, 0.01, 0.09, or 0.80 mg/m^3) for 6 hours/day, 5 days/week, for 1 year. The mass median aerodynamic diameter (MMAD) was 3.7 microns, and sigma g was 1.7 for all concentrations. Some animals were held for an additional 1-year recovery period and interim sacrifices were made at the end of 6 and 12 months during exposure as well as the end of the 6- and 12-month post-exposure recovery time. Lung clearance times were 2.3, 3.6, and 9.5 months for the low, mid-, and high-concentration groups, exposed animals retained 10.6, 120, and 1,460 micrograms/g lung tissue in the three exposure groups, respectively, after 1 year of exposure	IRIS, 2002; Newton et al., 1994	The antimony trioxide atmosphere for treated rats was generated using fluidizing bed generators; resulting dust-laden streams were then delivered into inhalation chambers.
		Hamsters were exposed to pure antimony trioxide (volume median diameter of 7.0 microns) or dust containing 1.6% antimony (by weight) via intratracheal instillation and lung clearance was determined. The half-life of elimination from hamster lungs was 20–40 days.	IRIS, 2002	Reported in a secondary source, limited study details provided.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Acute Mammalian Toxicity		**LOW: Antimony trioxide is considered of low acute toxicity for oral, dermal, and inhalation exposure.**		
Acute Lethality	**Oral**	No deaths were reported in rats administered antimony trioxide in food at ≤ 16,714 mg/kg-day	ATSDR, 1992	Reported in a secondary source, limited study details provided.
		Rat oral LD_{50} > 20,000 mg/kg	EU RAR, 2008	Reported in a secondary source
	Dermal	Rabbit dermal LD_{50} >8,300 mg/kg-bw	OECD SIAP, 2008	Reported in a secondary source, limited study details provided.
	Inhalation	Rat 4-hour LC_{50} >5,200 mg/m^3 dust (5.2 mg/L)	OECD SIAP, 2008	Reported in a secondary source, limited study details provided.
Carcinogenicity		**LOW: Based on the absence of carcinogenicity following inhalation to antimony trioxide dust in rats for 1 year. Inadequate inhalation studies reported a potential for lung tumors; however, these studies are considered unreliable due to study limitations and are not sufficient for determining a hazard designation. No data was located on the potential carcinogenicity of antimony trioxide to humans or on potential carcinogenicity to animals following oral or dermal exposure. A 2 year cancer bioassay is in progress at NTP.**		
	OncoLogic Results			No data located. This inorganic compound is not amenable to available estimation methods.
	Carcinogenicity (Rat and Mouse)			No data located.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Combined Chronic Toxicity/ Carcinogenicity	Wistar rats (45/sex/group) were exposed to 45 mg/m^3 antimony trioxide dust (duration-adjusted concentration = 9.4 mg/m^3; MMAD = 2.80) or 36–40 mg/m^3 antimony ore (duration-adjusted = 7.9 mg/m^3; MMAD = 4.78) up to 52 weeks at 7 hours/day, 5 days/week. Interim sacrifices were performed at 6, 9, and 12 months (5/sex/group) and the remaining animals were allowed to recover for 20 weeks. Slight decreases in body weight, and slightly raised white and yellow foci were observed on pleural surfaces in lung. After 6 months, all animals developed interstitial fibrosis, alveolar-wall cell hypertrophy, and hyperplasia, and cuboidal and columnar cell metaplasia of the lungs. The affected area increased in size after 12 months and the extent of fibrosis increased after 4–5 months recovery. An increased incidence (27%) of lung tumors (squamous-cell carcinomas, bronchoalveolar adenomas, bronchoalveolar carcinomas, and scirrhous carcinomas) was observed in females only, while no lung tumors were reported for controls.	Groth et al. 1986; IRIS, 2002	Reported in a secondary source, limited study details provided. Only one concentration was tested. Study conducted prior to the implementation of guideline studies developed from standardized methodologies. The chemical substance used in testing also contained detectable levels of arsenic, a known human carcinogen.

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Rats exposed via inhalation to 4.01 mg antimony/m^3 as antimony trioxide dust for 6 hours/day, 5 days/week, 1 year did not exhibit an increase the incidence of lung tumors.	Newton et al. 1994; ATSDR, 1992; IRIS, 2002	Reported in a secondary source, limited study details provided. Units measured as mg antimony/m^3 as antimony trioxide.
		Increased incidence of lung tumors were observed in female rats exposed to 4.2 or 36 mg antimony/m^3 as antimony trioxide dust 6 hours/day, 5 days/week, for 1 year.	Watt, 1980, 1983; ATSDR, 1992	Reported in a secondary source, limited study details provided. Units measured as mg antimony/m^3 as antimony trioxide. Only female rats were tested. Study conducted prior to the implementation of guideline studies developed from standardized methodologies.
Genotoxicity		**LOW: Antimony trioxide does not appear to cause gene mutations in bacteria or mouse lymphoma cells in *vitro*. While positive results were found *in vitro* for induction of sister chromatid exchange (SCE) in human lymphocytes and Chinese hamster V79 cells, *in vivo* inhalation exposure to mice and rats does not induce chromosomal aberrations and micronuclei. The potential for clastogenicity was reported *in vivo*; however, these studies are inadequate due to study limitations.**		
	Gene Mutation *in vitro*	Negative in two Ames tests using *Salmonella* strains TA1535, TA1537, TA100, TA98, and *E. coli* strains WP2PuvrA and WP2P.	EU RAR, 2008	Reported in a secondary source. Performed according to OECD Guideline 471 and GLP).
		Negative in the mouse lymphoma L5178Y mutation assay	EU RAR, 2008	Reported in a secondary source. Performed according to OECD Guideline 476 and GLP).
	Gene Mutation *in vivo*			No data located.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Chromosomal Aberrations *in vitro*	Positive in a cytogenetic assay using human lymphocytes isolated from two different donors, with and without metabolic activation.	EU RAR, 2008	Reported in a secondary source. Performed according to OECD Guideline 473 and GLP.
		Positive for inducing SCE in human lymphocytes and V79 Chinese hamster cells.	EU RAR, 2008	Reported in a secondary source.
	Chromosomal Aberrations *in vivo*	Positive in micronucleus bone marrow and peripheral blood assay in B6C3F1 male and female mice, inhalation exposure.	NTP, 2011	Reported in a secondary source. This study is not sufficient for determining a hazard designation because antimony trioxide appears to have effects on erythroid colony development.
		Negative for an increase in the incidence of micronuclei in CD-1 mice following single (5,000 mg/kg) or repeat (400, 667, or 1,000 mg/kg/day; males only) oral administration of antimony trioxide (bone marrow micronucleus assay)	EU RAR, 2008	Reported in a secondary source. Performed according to OECD Guideline 474 and GLP). No lethality reported.
		Negative in a chromosomal aberrations test in mouse bone marrow following single gavage administration of 400, 667 or 1,000 mg/kg bw to male and female Swiss albino mice (5/sex/group). Observations were made 6, 12, 18 and 24 hours post exposure.	EU RAR, 2008	Reported in a secondary source. No positive control was used and is inadequate for determining hazard designation.

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Positive in a chromosomal aberrations test in mouse bone marrow following repeated gavage administration of 400, 667 or 1,000 mg/kg bw to male Swiss albino mice (5/sex/group) daily for 21 days. Observations were made on days 7, 14, and 21. Frequencies of chromosomal aberrations were significantly increased in a dose dependent manner, but did not show a duration-dependent association.	EU RAR, 2008	Reported in a secondary source. Only male mice tested. Exposure to the highest dose was lethal by day 20 of treatment. No positive control was used. Lethality in this study was not seen in other studies at similar doses. Due to lethality, no chromosomal aberrations were evaluated in the high dose group on the day 21 observation. The EU RAR considers these results to be questionable due to the unexplained lethality in the high dose group, and inconsistencies in reporting.
		Negative for chromosome aberrations and micronuclei in the bone marrow of male and female Sprague-Dawley rats (6/group) administered 250, 500, or 1,000 mg/kg bw/day for 21 days. The mitotic index and percentage of polychromatic erythrocytes showed no evidence of bone marrow toxicity.	EU RAR, 2008	Reported in a secondary source. No lethality reported.
	DNA Damage and Repair	Positive in two *Bacillus subtilis* Rec assays using strains H17 (Rec^+) and M45 (Rec^-).	EU RAR, 2008	Reported in a secondary source.
		Negative in a rat liver unscheduled DNA synthesis study in male Alderly Park AlPk:ApfSD rats (5/dose) following a single oral dose of 3,200 or 5,000 mg/kg.	EU RAR, 2008	Performed according to OECD Guideline 486 and GLP.
	Other (Mitotic Gene Conversion)			No data located.

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Reproductive Effects		**LOW: There were no effects on reproductive organs in available repeated dose studies. However, there is uncertainty because the studies did not conduct a comprehensive evaluation of reproductive parameters. Reproductive effects following inhalation exposure to antimony trioxide cannot be ruled out at this time.**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Reproduction and Fertility Effects	Rats exposed to 250 mg antimony trioxide dust/m^3 for 4-hours/day beginning 3–5 days before estrus, through mating and gestation until 3-5 days before birth (total 63–78 days) had difficulty conceiving and delivered reduced numbers of offspring. LOAEC = 209 mg/m^3 (0.21 mg/L)	ATSDR, 1992; IRIS, 2002	Reported in secondary sources; a NOAEC was not identified. There is uncertainty as to the lowest concentration effects might occur. It is possible effects may occur at lower concentrations. Only one concentration was tested. Study conducted prior to the implementation of guideline studies developed from standardized methodologies.
		Changes in menstrual cycles, spontaneous late abortions, and early interruption of pregnancies were reported for female workers exposed to antimony dusts at an antimony metallurgical plant.	ATSDR, 1992; IRIS, 2002	Occupational exposures involving mixed compounds, undefined control group; reported in a secondary source, limited study details provided.
		Rat and Mouse, oral (gavage), 4-week repeated dose study; No effects on testicular toxicity. NOAEL = 1200 mg/kg-day (Highest dose tested)	OECD SIAP, 2008	Reported in a secondary source; study was not designed as a reproductive study; It was not specified if other reproductive parameters were examined.

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Wistar rats, male and female, dietary exposure 84–1879 mg/kg/day for 90 days. No effects in testes ≤ 1686 mg/kg-day; No effects in ovaries and uterus ≤ 1879 mg/kg-day. NOAEL = 1686 mg/kg/day (male) NOAEL = 1,879 mg/kg/day (female) LOAEL = not identified.	OECD SIAP, 2008	Reported in a secondary source, study details and test conditions were not provided. Did not conduct a comprehensive evaluation of reproductive parameters, but did examine reproductive organs. Sources cited four significant figures in results.
Developmental Effects		**LOW: Low potential for developmental effects based on expert judgment. Available data are insufficient to determine a hazard designation for this endpoint. The highest concentration tested was identified as a NOAEC (0.0063 mg/L), but a LOAEC was not identified. It is possible that effects could occur at concentrations that could be designated as a hazard concern if tested at higher concentrations.**		
	Reproduction/ Developmental Toxicity Screen	Low potential for developmental effects. (Estimated)	Expert judgment	Estimated based on expert judgment.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Prenatal Development	Rats (strain not specified; 26 females/group) received 0, 1.5, 3.0, or 6.0 mg/m^3 antimony trioxide (actual concentrations delivered: 2.6, 4.4, or 6.3 mg/m^3) by nose-only inhalation on gestational days (GD) 0 through 19 (6 hours/day). Particle size ranged from 1.59 - 1.82 microns. No mortalities and no treatment-related effects in the dams were reported for clinical signs, body weight change, or food consumption. No evidence of fetotoxicity was observed on GD 20 for implantation rate, fetal sex ratios, fetal body weights or crown-rump length, or fetal external, visceral, or skeletal examinations. Maternal gross examination revealed no treatment-related effects for clinical signs, food consumption or body weight changes; however, histopathologic examination found increased lung weight (24%, 31%, and 39% over controls at 2.6, 4.4, or 6.3 mg/m^3, respectively) at every dose level, with diffuse accumulation of pigmented alveolar macrophages, likely due to phagocytosis and accumulation of particulate matter of the test substance. NOAEC developmental = 6.3 mg/m^3 (0.0063 mg/L, highest dose tested) LOAEC developmental = not established NOAEC maternal toxicity = not established LOAEC maternal toxicity = 2.6 mg/m^3 (0.0026 mg/L)	International Antimony Oxide Industry Association, 2004	Reported in secondary source; a LOAEL for developmental toxicity was not identified in the study. The highest dose tested did not result in developmental effects.

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Increased incidence of spontaneous abortions in female workers at an antimony metallurgy plant.	ATSDR, 1992	Reported in a secondary source, limited study details provided. Occupational exposures involving mixed compounds, undefined control group.
	Postnatal Development			No data located.
Neurotoxicity		**LOW: Potential for neurotoxicity based on professional judgment. The experimental LOAEL values (6,544 mg/kg-day) for dogs and rabbits fall into the LOW hazard criteria range.**		
	Neurotoxicity Screening Battery (Adult)			No data located.
	Developmental Neurotoxicity			
	Other Neurotoxicity			
		Dogs developed muscle weakness and difficulty moving the hind limbs when administered antimony trioxide by gavage for 32 days. LOAEL = 6,544 mg/kg/day (only dose tested)	ATSDR, 1992	Reported in a secondary source, no study details and test conditions provided. A NOEL was not identified. There is uncertainty as to the lowest dose effects might occur. It is possible effects may occur at lower doses that would warrant a moderate or high hazard designation.
		Abnormal gait was observed in rabbits following a single dermal application LOAEL= 6,685 mg/kg/day (only dose tested).	ATSDR, 1992	Reported in a secondary source, limited study details provided. This was a lethal dose in the range finding study. A NOEL was not identified. There is uncertainty as to the lowest dose effects might occur. It is possible effects may occur at lower doses that would warrant a moderate or high hazard designation.

Antimony Trioxide CASRN 1309-64-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects	**MODERATE: Based on experimental studies in which lung overload was reported. Toxicity following inhalation of antimony trioxide dust is due to impaired lung clearance and particle overload followed by inflammatory responses and fibrosis. LOAEC values indicate a low concern for repeated dose effects following oral administration and toxicokinetic studies indicate that antimony trioxide is poorly absorbed when administered orally. A 2-year inhalation cancer bioassay in rats and mice is in progress at NTP.**		
	Several occupational studies examined mine and smelter workers exposed to airborne dust concentrations of up to 138 mg/m^3 antimony trioxide (0.138 mg/L), and particle size averaging <5 mm, concentrated in the mid lung region. A common finding in the subjects examined was antimony pneumoconiosis characterized by diffuse, densely distributed punctuate opacities, having a round, polygonal or irregular shape, and averaging <1 mm diameter.	IRIS, 2002	Reported in a secondary source; occupational exposures to airborne mixtures of antimony trioxide and/or pentoxide.

Antimony Trioxide CASRN 1309-64-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	24 guinea pigs were exposed to 45.4 mg/m^3 antimony trioxide dust (approximately 38.1 mg antimony/m^3) 2 hours/day, 7 days/week for 2 weeks followed by 3 hours/day for 8–265 days. Particle size was assumed to be <1 micron. Necropsy revealed increased lung weight, interstitial pneumonitis, and subpleural petechial hemorrhages in animals exposed for ≥ 30 days. Increased liver weight, fatty degeneration, and cloudy swelling of the liver were noted in animals exposed for ≥48 days, and decreased white blood counts and splenic hypertrophy and hyperplasia were seen in about 50% of the exposed animals. LOAEC = 45.4 mg/m^3 (0.045 mg/L)	IRIS, 2002	Reported in a secondary source, study details and test conditions were not provided. Only one concentration tested. Study conducted prior to the implementation of guideline studies developed from standardized methodologies.
	Inhalation exposure of rats, 6 hours/day, 5 day/week ≥ 13 weeks resulted in proliferation of alveolar macrophages. LOAEC = 0.92 mg/m^3 (0.00092 mg/L)	ATSDR, 1992	Reported in a secondary source, study details and test conditions were not provided. Study conducted prior to the implementation of guideline studies developed from standardized methodologies.
	Dogs developed severe diarrhea and muscle weakness when administered antimony trioxide by gavage for 32 days. LOAEL = 6,544 mg/kg/day	ATSDR, 1992	Reported in a secondary source, study details and test conditions were not provided.

Antimony Trioxide CASRN 1309-64-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Fischer 344 rats (50/sex/group) were exposed to target concentrations of 0, 0.2, 1.0, 5.0, or 25.0 mg/m^3 (actual concentrations were 0, 0.25, 1.08, 4.92, or 23.46 mg/m^3) for 6 hours/day, 5 days/week, 13 weeks (duration-adjusted concentrations = 0, 0.05, 0.19, 0.88, or 4.20 mg/ m^3, respectively). Interim sacrifices (5/sex/group) were conducted at weeks 1, 2, 4, 8, and 13, and some animals were held an additional 27 weeks for recovery. Complete gross and histopathological examinations were conducted on all animals, while hematology and clinical chemistry analysis were performed for 5/sex/group at exposure and recovery weeks 1,2,4,8, and 13. Body weight in males and females was reduced at the two highest concentrations, and mean and absolute lung weights were increased in both sexes at the two highest concentrations during exposure and early part of recovery. Gross necropsy revealed discolored lungs and microscopic examination found particle-laden and degenerating macrophages, cellular debris in the lumen of the alveoli, pneumatocyte hyperplasia, and alveolar wall thickening, which were still present at week 27 of recovery. NOAEL = 1.08 mg/m^3 (0.001 mg/L) LOAEL = 4.92 mg/m^3 (0.0049 mg/L)	Newton et al., 1994; IRIS, 2002	Reported in a secondary source.

Antimony Trioxide CASRN 1309-64-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Fischer 344 rats (65/sex/group) were exposed (whole-body) to antimony trioxide at target concentrations of 0, 0.05, 0.5, or 5.0 mg/m^3 (duration-adjusted concentrations: 0, 0.01, 0.09, or 0.80 mg/ m^3) for 6 hours/day, 5 days/week, 1 year. Some animals were held for an additional 1-year recovery period and interim sacrifices were made at the end of 6 and 12 months during exposure as well as the end of the 6- and 12-month post-exposure recovery time. Gross and histopathological examinations were conducted on all animals and hematology analyses were performed on subgroups at 12, 18, and 24 months. Ophthalmoscopic evaluation found an 11, 2, 28 and 32% increased incidence of cataracts from lowest to highest test concentration, respectively. Interstitial inflammation and granulomatous inflammation were observed at all concentrations. Statistical analysis indicated a significant increase in incidence and severity in these effects at the high-exposure in both sexes. Pulmonary clearance was decreased by 80% in the high-concentration group and the clearance halftime was increased from 2 months to 10 months. LOAEL = 0.05 mg/m^3 (0.0005 mg/L)	Newton et al., 1994; IRIS, 2002	Reported in a secondary source, not a guideline study.

Antimony Trioxide CASRN 1309-64-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Wistar rats (50 females/group) and Sinclair S-1 miniature pigs (3 females/group) to 0, 1.9, or 5.0 mg/m^3 (duration-adjusted concentrations = 0, 0.3, and 0.9 mg/m^3, respectively) antimony trioxide for 6 hours/day, 5 days/week, 1 year. Particle size was 0.44 and 0.40 microns for the low and high concentrations, respectively. Survival, hematology and clinical chemistry were not affected by exposure for either species. Lung weights were increased and pulmonary focal fibrosis, adenomatous hyperplasia, multinucleated giant cells, cholesterol clefts, pneumonocyte hyperplasia, and pigmented macrophages were observed. Necropsy revealed pulmonary discoloration and increased alveolar-intralveolar macrophages in both exposure groups, while focal subacute-chronic interstitial inflammation and granulomatous inflammation observed in the high-exposure group. LOAEL = 1.9 mg/m^3 (0.0019 mg/L, lowest concentration tested)	IRIS, 2002	Reported in a secondary source. Study conducted prior to the implementation of guideline studies developed from standardized methodologies.

Antimony Trioxide CASRN 1309-64-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Wistar rats, male and female, dietary exposure of 0, 1,000, 5,000, or 20,000 ppm (male: 0, 84, 421, 1,686 mg/kg-day; female: 0, 97, 494, 1,879 mg/kg-day) for 90 days. In high-dose males: increased triglycerides, red blood cells (RBC), and urine volume; decreased alkaline phosphatase activity. In high-dose females: increased RBC, urine volume, serum cholesterol, and aspartate and alanine aminotransferase; decreased alkaline phosphatase activity (mid-dose too) and urine specific gravity. NOAEL = 94 mg/kg/day LOAEL = 20,000 ppm (1,879 and 1,686 mg/kg/day in females and males, respectively)	NTP, 2005	Reported in a secondary source.
	Male Wistar rats, dietary exposure, 500 or 1,000 mg antimony trioxide/kg/day, 24 weeks. Decreased red blood cell count; increased serum glutamic oxaloacetic transaminase LOAEL=500 mg/kg/day	NTP, 2005	Reported in a secondary source, study details and test conditions were not provided.
	Rats (strain and sex not given), dietary exposure, 670 mg antimony trioxide/kg/day, 12 weeks. Decreased weight gain, spleen weight, and heart weight; increased lung weight LOAEL = 670 mg/kg/day (only dose tested)	NTP, 2005	Reported in a secondary source, study details and test conditions were not provided.

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Rats (strain and sex not given), dietary exposure, 420–490 mg antimony trioxide/kg/day, 24 weeks. Decreased weight gain, decreased RBC and cloudy swelling in hepatic cords. LOAEL = 418 mg/kg/day	ATSDR, 1992; NTP, 2005	Reported in a secondary source, study details and test conditions were not provided.
Skin Sensitization		**LOW: Antimony trioxide was not sensitizing in guinea pigs.**		
	Skin Sensitization	Not sensitizing to guinea pigs.	OECD SIAP, 2008	Reported in a secondary source, limited study details provided.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Antimony trioxide is mildly irritating to rabbit eyes.**		
	Eye Irritation			
		Instillation of 34.5–83.6 mg antimony (as antimony trioxide) into the eyes of rabbits did not produce irritation.	ATSDR, 1992	Reported in a secondary source, limited study details provided.
		Two studies showed reversible mild eye irritation in rabbits.	OECD SIAP, 2008	Reported in a secondary source, limited study details provided.
Dermal Irritation		**MODERATE: Antimony trioxide is reported to produce skin irritation in workers, but no data were located regarding skin irritation studies in animals.**		
	Dermal Irritation	Human case study reports have indicated that antimony trioxide may cause dermatitis on damp skin; irritation associated with sweat ducts.	OECD SIAP, 2008	Reported in a secondary source, human case study reports.
Endocrine Activity		**No data located.**		
				No data located.

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Immunotoxicity		**Inhalation exposure to antimony trioxide caused decreased white blood counts and splenic hypertrophy and hyperplasia in guinea pigs.**		
	Immune System Effects	24 guinea pigs were exposed to 45.4 mg/m^3 antimony trioxide dust (approximately 38.1 mg antimony/m^3) 2 hours/day, 7 days/week for 2 weeks followed by 3 hours/day for 8–265 days. Particle size was assumed to be <1 micron. Decreased white blood counts and splenic hypertrophy and hyperplasia were seen in about 50% of the exposed animals. LOAEC = 45.4 mg/m^3 (0.045 mg/L)	IRIS, 2002	Reported in a secondary source, no study details and test conditions were provided. Only one concentration tested.
ECOTOXICITY				
ECOSAR Class		Not applicable.		
Acute Toxicity		**MODERATE: Based on an experimental acute toxicity value for fish. The acute toxicity value of 1.77 mg Sb/L in *Chlorohydra viridissima* would indicate a HIGH hazard designation; however, this species may not be suitable for determining hazard designations. Other experimental aquatic toxicity values for fish and daphnia exceed the water solubility of the compound suggesting no effects at saturation.**		
Fish LC_{50}		*Lepomis macrochirus* 96-hour LC_{50} >530 mg/L	ECOTOX	Inadequate; data exceeds measured water solubility of compound; limited data make it difficult to determine whether the data refer to antimony ion or antimony trioxide.
		Danio rerio 96-hour LC_{50} >1,000 mg/L	IUCLID, 2000	Inadequate; data exceeds measured water solubility of compound; limited data make it difficult to determine whether the data refer to antimony ion or antimony trioxide.

Antimony Trioxide CASRN 1309-64-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Pimephales promelas 96-hour LC_{50} > 80 mg/L	ECOTOX	Inadequate; data exceeds measured water solubility of compound; limited data make it difficult to determine whether the data refer to antimony ion or antimony trioxide.
	Pimephales promelas 96-hour LC_{50} = 14.4 mg Sb/L	EU RAR, 2008	Reported in a secondary source. Test substance identified as $SbCl_3$.
	Pagrus major 96-hour LC_{50} = 12.4 mg Sb/L	EU RAR, 2008	Reported in a secondary source. Test substance identified as $SbCl_3$.
Daphnid LC_{50}	*Daphnia magna* 48-hour EC_{50} = 423 mg/L	ECOTOX	Inadequate; data exceeds measured water solubility of compound; limited data make it difficult to determine whether the data refer to antimony ion or antimony trioxide.
	Daphnia magna 48-hour EC_{50} >1,000 mg/L	IUCLID, 2000	Inadequate; data exceeds measured water solubility of compound; limited data make it difficult to determine whether the data refer to antimony ion or antimony trioxide.
	Daphnia magna 48-hour LC_{50} = 12.1 mg Sb/L	EU RAR, 2008	Reported in a secondary source.
	Chlorohydra viridissima (hydra), 96-hour LC_{50} = 1.77 – 1.95 mg Sb/L; measured filtered)	EU RAR, 2008	Reported in a secondary source. Test substance identified as $SbCl_3$
Green Algae EC_{50}	*Pseudokirchneriella subcapitata* 72-hour EC_{50} = 0.73 mg /L (based on chlorophyll A concentration)	ECOTOX	Inadequate; reported in a secondary source; not a traditional endpoint for determining hazard concern; *Pseudokirchneriella subcapitata* is, more recently known as *Raphidocelis subcapitata.*

Antimony Trioxide CASRN 1309-64-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Raphidocelis subcapitata 72-hour EC_{50} > 36.6 mg Sb/L (growth rate) NOEC = 2.11 mg Sb/L	EU RAR, 2008	Reported in a secondary source. Test substance identified as $SbCl_3$
	Raphidocelis subcapitata 72-hour EC_{50} > 2.4 mg Sb/L (growth rate) NOEC = 0.396 mg Sb/L LOEC = 1.32 mg Sb/L	EU RAR, 2008	Reported in a secondary source. Test substance identified as Sb_2O_3
	Lemma minor 96-hour EC_{50} > 25.5 mg Sb/L; NOEC = 12.5 mg Sb/L LOEC = 25.5 mg Sb/L (reduction in frond production)	EU RAR, 2008	Reported in a secondary source. Test substance identified as $SbCl_3$
Chronic Aquatic Toxicity	**MODERATE: Based on experimental LOECs ranging from 2.31 to 4.50 mg Sb/L in fish and daphnia.**		
Fish ChV	*Pimephales promelas* 28-day NOEC= 2.31 mg/L; LOEC 4.50 mg Sb/L (growth – weight)	EU RAR, 2008	Reported in a secondary source. Test substance identified as $SbCl_3$
	Pimephales promelas 28- day NOEC= 1.13 mg/L (growth – length); LOEC = 2.31 mg Sb/L.	EU RAR, 2008	Reported in a secondary source. Test substance identified as $SbCl_3$
	Pimephales promelas 28- day NOEC >0.0075 mg Sb/L (growth)	EU RAR, 2008	Reported in a secondary source. There were no effects reported at the highest dose tested. Test substance identified as Sb_2O_3
Daphnid ChV	*Daphnia magna* 21-day NOEC = 1.74 mg Sb/L; LOEC = 3.13 mg Sb/L	EU RAR, 2008	Reported in a secondary source. Test substance identified as $SbCl_3$
	Daphnia ChV = 3.8 mg/L (Estimated)	EPI; Professional judgment	Based on SARs (not computerized) developed for confidential antimony salts.
Green Algae ChV			No data located.
ENVIRONMENTAL FATE			

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Transport		**The limited mobility observed under experimental conditions and the low vapor pressure indicates that antimony trioxide is anticipated to partition predominantly to soil and sediment. It will not volatilize from water. Soil mobility and sediment adsorption tests indicate that antimony trioxide will be immobile in soil, and therefore will not be expected to migrate into groundwater.**		
	Henry's Law Constant(atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment	Cutoff value for non volatile compounds. This inorganic compound is not amenable to available estimation methods.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	No significant evidence of mobility in sand, clay, or sandy and silt loams when tested at 100-µL concentration after 24 hours (Non-TSCA Protocol/Guideline) (Measured)	EPA, 2006; EPA, 2011	Although not a guideline study, the data suggest that antimony trioxide will have a K_{oc} above >30,000, the SF guidance cutoff value for non-mobile substances.
	Level III Fugacity Model			Not all input parameters for this model were available to run the estimation software (EPI).
Persistence		**HIGH: Antimony trioxide is an inorganic substance containing metallic atoms that are likely to be found in the environment for more than 180 days after release, resulting in a very high persistence hazard assignment. Based on water solubility studies under a range of pH values, antimony trioxide is expected to slowly dissolve resulting in the release of antimony ions and, depending on pH, be oxidized or reduced to other oxidation states. Additionally, results from a pure culture study using autotrophic bacterium indicate that antimony may be oxidized by bacteria. Antimony trioxide is not anticipated to undergo hydrolysis under environmental conditions. Antimony trioxide does not contain functional groups expected to absorb light at environmentally significant wavelengths, and therefore is not expected to photolyze. No degradation processes for antimony trioxide under typical environmental conditions were identified.**		
Water	**Aerobic Biodegradation**			No data located.
	Volatilization Half-life for Model River			No data located.
	Volatilization Half-life for Model Lake			No data located.

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Soil	**Aerobic Biodegradation**	Autotrophic bacteria, *Stibiobacter senarmontii*, were grown in a mineral medium containing antimony trioxide during a pure culture study. Antimony trioxide was oxidized at rates of 45.5–51.6 and 13.5–19.3 mg/month for senarmonite and valentinite, respectively; little oxidation occurred in the sterile medium. (Measured)	EPA, 1985	Nonguideline study that demonstrated that the half-life of antimony trioxide is anticipated to be >180 days.
	Anaerobic Biodegradation			No data located.
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation	10 and 100 ppm antimony trioxide with added nutrients were incubated with natural bottom sediment from Puget Sound under aerobic or anaerobic conditions for up to 120 days. Three organoantimony biotransformation products were found in solution after 60 days. Two of these were identified as methylstibonic acid and dimethylstibonic acid. No determination of rate or conditions affecting the transformation was made. However, it was estimated that much less than 0.1% of the antimony present was transformed. (Measured)	ATSDR, 1992	Nonguideline study reported in a secondary source that demonstrated limited biodegradation.
Air	**Atmospheric Half-life**			No data located.

Antimony Trioxide CASRN 1309-64-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
	Hydrolysis	Reacts with acids producing Sb^{3+} compounds and bases producing $[Sb(OH)_4]^-$ (Measured)	Umwelt Bundes Amt, 2001	Although hydrolysis may occur upon contact with strong acids or bases, these data do not address the potential for hydrolysis under environmental conditions.
Environmental Half-Life		>180 days (Estimated)	Professional judgment	Antimony trioxide is an inorganic compound. Antimony ions, oxides, or hydroxides are expected to be found in the environment >180 days after release.
Bioaccumulation		**LOW: Antimony trioxide is an inorganic compound and is not expected to bioaccumulate.**		
	Fish BCF	<100 (Estimated)	Professional judgment	Antimony oxide is an inorganic compound and is not anticipated to bioaccumulate or bioconcentrate. This inorganic compound is not amenable to available (Q)SAR models.
		No reliable bioaccumulation or bioconcentration studies located.	OECD SIAP, 2008	
	BAF	<100 (Estimated)	Professional judgment	
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		Antimony trioxide has been detected in dust samples collected downwind from a copper smelting plant in Washington state (Crecelius et al., 1975). Antimony is thought to oxidize to antimony trioxide in combustion and incineration processes (EU RAR, 2008). Antimony trioxide is found naturally occurring in ores such as senarmonite, valentinite and exitelite (Canada, 2010).		
Ecological Biomonitoring		No data located.		

Antimony Trioxide CASRN 1309-64-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Human Biomonitoring	Women working in an antimony metallurgical plant, exposed to unspecified amounts of antimony trioxide, metallic antimony, and antimony pentasulfides were compared with a similar group of women not exposed to antimony. The plant workers had ten times the antimony concentration in their blood compared to controls; additional sampling performed on urine, breast milk, placental tissue, amniotic fluid and umbilical cord blood samples (EPA, 1985). This chemical was not included in the NHANES biomonitoring report (CDC, 2011). Additionally, it was reported that antimony has been found in fetal liver as well as in human breast milk, placenta, amniotic fluid and umbilical cord blood (EU RAR, 2008).		

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Bis(hexachlorocyclopentadieno) Cyclooctane

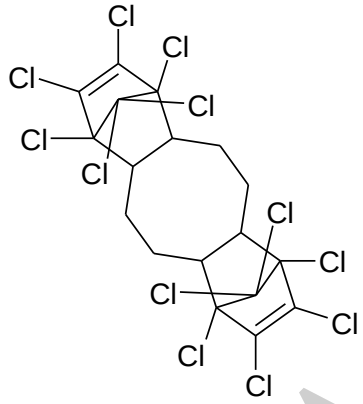
Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.
§ Based on analogy to experimental data for a structurally similar compound.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Bis(hexachlorocyclopentadieno) Cyclooctane	13560-89-9	L	*M*§	*M*§	VL	VL	L	M	L		VL	*L*	*L*	*L*	VH	*H*

Bis(hexachlorocyclopentadieno) Cyclooctane



CASRN: 13560-89-9

MW: 653.73

MF: $C_{18}H_{12}Cl_{12}$

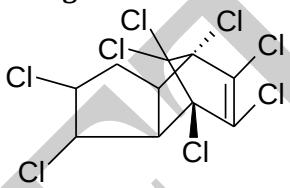
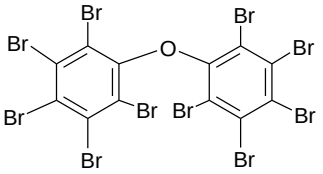
Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: C(=C(C(C1(Cl)Cl)(C(C2CCC(C(C(=C(C34Cl)Cl)Cl)(C3(Cl)Cl)Cl)C4C5)C5)Cl)Cl)(C12Cl)Cl

Synonyms: 1,4:7,10-Dimethanodibenzo[a,e]cyclooctene, 1,2,3,4,7,8,9,10,13,13,14,14-dodecachloro-1,4,4a,5,6,6a,7,10,10a,11,12,12a-dodecahydro- (TSCA Inventory); 1,2,3,4,7,8,9,-10,13,13,14,14-Dodecachloro-1,4,4a,5,6,6a,7,10,10a,11,12,12a-dodechydro-1,4:7,10-dimethanodibenzo[a,e]cyclooctene; 1,4:7,10-Dimethanodibenzo(a,e)cyclooctene,1,2,3,4,7,8,9,10,13,13,14,14-dodecachloro-1,4,4a,5,6,6a,7,10,10a,11,12,12a-dodecahydro-; 1,6,7,8,9,14,15,16,17,17,18,18-Dodecachloropentacyclo(12.2.1.16,9.02,13.05,10)octadeca-7,15-diene; Bis(hexachlorocyclopentadieno)cyclooctane; Dechloran A; Dechlorane 605; Dechlorane Plus; Dechlorane Plus 1000; Dechlorane Plus 25; Dechlorane Plus 2520; Dechlorane Plus 35; Dechlorane Plus 515; Dodecachlorododecahydrodimethanodibenzocyclooctane; Dodecachlorododecahydrodimethanodibenzocyclooctene; Dodecachloropenta-cycloctadeca-7,15 diene

Chemical Considerations: This is a discrete organic chemical with a MW below 1,000. EPI v 4.0 was used to estimate physical/chemical and environmental fate values due to an absence of experimental data. Measured values from experimental studies were incorporated into the estimations.

Polymeric: No **Oligomers:** Not applicable	
Metabolites, Degradates and Transformation Products: None	
Analogs: Chlordane (57-74-9), decabromodiphenyl ether (1163-19-5, organochlorine pesticides, and confidential structures **Endpoint(s) using analog values:** Carcinogenicity, Genotoxicity, Repeated Dose	**Analog Structures:**  Chlordane (57-74-9)  Decabromodiphenyl ether (1163-19-5)
Structural Alerts: Aliphatic halogenated hydrocarbons, cyclic halogenated hydrocarbons for neurotoxicity, and chlorinated hydrocarbons for reproductive toxicity (U.S. EPA, 2011a).	
Risk Phrases: Not classified by Annex I Directive 67/548/ EEC & IUCLID (Pakalin, 2007).	
Hazard and Risk Assessments: Risk assessment completed for bis(hexachlorocyclopentadieno) cyclooctane by the European Chemicals Bureau in 2007 (Pakalin, 2007).	
U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.	

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	Decomposes at 350°C (Measured)	Occidental Chemical Company, 2009	Material decomposes before melting.
Boiling Point (°C)	Decomposes at 350°C (Measured)	Occidental Chemical Company, 2009	Material decomposes before boiling.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	EPI; EPA, 2011b	Cutoff value for nonvolatile compounds according to SF assessment guidance.
	0.006 at 200°C (Measured)	Occidental Chemical Company, 2009	Value reported at an elevated temperature.
Water Solubility (mg/L)	$4.4x10^{-5}$ (Measured)	Occidental Chemical Company, 2009	Adequate, nonguideline study.
	$2.49x10^{-4}$ (Measured)	Occidental Chemical Company, 2009	
	$2.07x10^{-4}$ to $5.72x10^{-4}$ (Measured)	Chou et al., 1979	
Log K_{ow}	>10 (Estimated)	EPI; EPA, 2011b	Cutoff value used according to SF assessment guidance.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize in environmental conditions.
pK_a	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize in environmental conditions.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**As a neat material, bis(hexachlorocyclopentadieno) cyclooctane is estimated to not be absorbed through the skin and it is also estimated to have poor skin absorption when in solution. This compound is expected to be poorly absorbed via the lungs and gastrointestinal tract. Bis(hexachlorocyclopentadieno) cyclooctane is not easily absorbed in the gastrointestinal tract with 93-98% of an administered dose excreted through the feces unchanged. Plasma levels peaked at 10 hours after administration; the highest levels of bis(hexachlorocyclopentadieno) cyclooctane were found in the liver, where metabolism is thought to take place, and in the ovaries. Bis(hexachlorocyclopentadieno) cyclooctane is excreted slowly if it is absorbed.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal, or Inhaled**	Not absorbed through the skin as the neat material; poor skin absorption if in solution; poor absorption from the lung and gastrointestinal tract. (Estimated)	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/chemical properties.
		In a toxicokinetic study, most excretion occurred through the feces unchanged (93-98%), less than 0.1% was excreted in urine and 0.004% excreted in expired air; plasma levels peaked at 10 hours, and tissue levels did not increase proportionally with dose; after 4 days, 26% of radiolabeled chemical was remaining in carcass; the highest levels were found in the ovaries and liver.	IUCLID, 2003	Guideline study.
	Oral	In a toxicokinetic study in rats, very little of the chemical is absorbed in the gastro-intestinal tract; 95% of administered radioactive dose was excreted in the feces; the small amount of chemical that did absorb was then excreted slowly; after absorption, the highest amount was found in the liver where metabolism takes place.	Chou et al., 1979	Unpublished study, but sufficient study details reported.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Acute Mammalian Toxicity		**LOW: Based on the acute oral and dermal toxicity values >3,160 mg/kg in rats and >8,000 mg/kg in rabbits, respectively. Although the acute inhalation study in rats produced no deaths, the LC_{50} value of >2.25 mg dust/L air (highest concentration tested) was not included in the hazard call because there is uncertainty regarding the potential for adverse effects between 2.25 and 5 mg/L.**		
Acute Lethality	**Oral**	Rat (Shermal-Wistar) oral LD_{50} >25,000 mg/kg; no mortalities at highest dose tested (25,000 mg/kg)	IUCLID/Occidental Chem Corp., 1992	Not specified as a guideline study, but follows general OECD guidelines.
		Rat (Sprague-Dawley) oral LD_{50} >3,160 mg/kg; no mortalities at the highest dose tested (3,160 mg/kg)	IUCLID, 2003	Not specified as a guideline study and reported in a secondary source, but follows general OECD guidelines.
	Dermal	Rabbit dermal LD_{50} >8,000 mg/kg; no mortalities at highest dose tested (8,000 mg/kg)	IUCLID/Occidental Chem Corp., 1992	Not specified as a guideline study, but follows general OECD guidelines.
	Inhalation	Rat inhalation 1-hour LC_{50} >300 mg dust /L air; no mortalities at highest dose tested (300 mg dust /L air)	IUCLID, 2003	Limited study details reported in a secondary source; not the preferred 4-hour exposure.
		Rat inhalation 4-hour LC_{50} >2.25 mg dust/L air (2,250 mg/m^3); no mortalities at highest dose tested (2.25 mg dust/L air)	IUCLID/Occidental Chem Corp., 1992	Not specified as a guideline study, but follows general OECD guidelines.
Carcinogenicity		**MODERATE: There is potential for carcinogenicity based on analogy to chlordane and decabromodiphenyl ether, the latter for expression of adverse effects in longer term studies. No carcinogenicity data regarding exposure to Bis(hexachlorocyclopentadieno) cyclooctane located.**		
	OncoLogic Results			Not amenable to available estimation method.
	Carcinogenicity (Rat and Mouse)	There is potential for oncogenicity. (Estimated by analogy)	Professional judgment	Estimated by analogy to chlordane.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Potential for carcinogenicity; increased incidence of neoplastic nodules of the liver in rats; equivocal evidence of increased incidences of hepatocellular adenomas or carcinomas and thyroid gland follicular cell adenomas or carcinomas in male mice. (Estimated by analogy)	Professional judgment	Estimated based on the high potential for bioaccumulation and by analogy to observations on decabromodiphenyl ether where adverse effects were not present in 90-day studies but were expressed following chronic exposure in a NTP study.
	Combined Chronic Toxicity/ Carcinogenicity			No data located.
Genotoxicity		**MODERATE: There is estimated to be an uncertain potential for mutagenicity based on analogy to chlordane. Bis(hexachlorocyclopentadieno) cyclooctane did not cause mutations in bacterial cells or mammalian cells *in vitro*. A moderate hazard designation is assigned because of the uncertain potential for genotoxicity based on chlordane and because there were no data located regarding the potential for bis(hexachlorocyclopentadieno) cyclooctane to cause chromosomal aberrations.**		
	Gene Mutation *in vitro*	Uncertain potential for mutagenicity (Estimated by analogy)	Professional judgment	Estimated by analogy to chlordane.
		Negative, Ames assay in *Salmonella typhimurium* strains TA98, TA100, TA1535, TA1537, TA1538 with and without metabolic activation.	IUCLID, 2003	Not specified as a guideline study and reported in a secondary source, but follows general OECD guidelines.
		Negative, Mouse lymphoma assay in L5178Y TK +/- cells with and without metabolic activation.	IUCLID, 2003	Not specified as a guideline study and reported in a secondary source, but follows general OECD guidelines.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*			No data located.
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair			No data located.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**VERY LOW: Bis(hexachlorocyclopentadieno) cyclooctane did not cause reproductive effects at oral doses as high as 5,000 mg/kg-day in a combined repeated dose/reproduction/developmental toxicity study in rats.**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	No adverse effects were observed in an oral (gavage) developmental and reproductive toxicity study in male and female rats (exposure to males: 21 days premating, 14 day mating period, and 28 days after completion of mating period; exposure to females: 21 days premating, 14 days mating, and up to 25 days after mating [GD 0 – LD 3]; no effects on reproductive or fertility indices through LD 4, and no effects on implantation or fetal indices through GD 20. NOEL = 5,000 mg/kg-day (highest dose tested)	Brock et al., 2010	Guideline study (OECD 422).
	Reproduction and Fertility Effects			No data located.
Developmental Effects		**VERY LOW: Bis(hexachlorocyclopentadieno) cyclooctane did not cause developmental effects at oral doses as high as 5,000 mg/kg-day in a combined repeated dose/reproduction/developmental toxicity study in rats.**		
	Reproduction/ Developmental Toxicity Screen			No data located.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	No adverse effects were observed in an oral (gavage) developmental and reproductive toxicity study in male and female rats (exposure to males: 21 days premating, 14 day mating period, and 28 days after completion of mating period; exposure to females: 21 days premating, 14 days mating, and up to 25 days after mating [GD 0–LD 3]; no effects on fetal development through LD 4, and no effects on external and visceral examinations through GD 20. NOEL = 5,000 mg/kg-day (highest dose tested)	Brock et al., 2010	Guideline study (OECD 422).
	Prenatal Development			No data located.
	Postnatal Development			No data located.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Neurotoxicity		**LOW: Bis(hexachlorocyclopentadieno) cyclooctane did not cause neurotoxic effects at oral doses as high as 5,000 mg/kg-day in a combined repeated dose/reproduction/developmental toxicity study in rats.**		
	Neurotoxicity Screening Battery (Adult)	No adverse effects were observed in a 28-day oral (gavage) study in male and female rats; no effects observed in FOB evaluations (activity/arousal, autonomic, neuromuscular, physiological, and sensimotor); a significant lower frequency of urination was observed in females exposed to 750 and 5,000 mg/kg-day, but was not considered biologically significant; a significant increase in rearing counts for males exposed to 1,500 mg/kg-day during 20-30-min. trials, but was considered not to be treatment related. NOEL = 5,000 mg/kg-day (highest dose tested)	Brock et al., 2010	Guideline study (OECD 422).

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects	**MODERATE: Bis(hexachlorocyclopentadieno) cyclooctane caused adverse liver and lung effects in rats following inhalation exposure to 0.64 mg dust/L (lowest concentration tested). No NOAEL was identified in this study so it is possible that effects could occur at lower concentrations. Bis(hexachlorocyclopentadieno) cyclooctane did not cause systemic effects at oral doses up to 5,000 mg/kg-day in a 28-day combined repeated dose/reproduction/developmental toxicity study in rats, in a 90-day dietary exposure study in rats at concentrations up to 100,000 ppm in the diet, or in a 28-day dermal exposure study in rabbits at doses up to 2,000 mg/kg-day.** **There is potential for chloracne estimated by analogy to organochlorine pesticides and potential for systemic effects estimated based on the high potential for bioaccumulation and potential for expression of adverse effects in longer term studies by analogy to decabromodiphenyl ether.**		
	There is a potential for chloracne. (Estimated by analogy)	Professional judgment	Estimated by analogy to organochlorine pesticides.
	No adverse effects were observed in a 28-day oral (gavage) study in male and female rats; no effects on in-life parameters (clinical signs, food consumption, body weight), clinical pathology (hematology, coagulation, clinical chemistry), or anatomic pathology (organ weight, abnormalities, microscopic). NOEL = 5,000 mg/kg-day (highest dose tested)	Brock et al., 2010	Guideline study (OECD 422).

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	In a 28-day inhalation (dust) study (6 hour/day, 5 day/week) in rats, a significantly increased absolute liver weight with hepatocytomegaly of centrilobular hepatocytes, increased absolute lung weights, and increased numbers of macrophages in the alveoli in both males and females were observed. There were no effects on body weight, signs of toxicity, urinalysis, hematology, clinical chemistry, or gross pathology. LOAEC = 0.64 mg/L (lowest concentration tested)	IUCLID/Occidental Chem Corp. 1992	Not specified as a guideline study, but follows general OECD guidelines.
	In a 90-day oral (dietary) study in rats, there were no significant treatment-related effects observed; no effects on body or organ weights, urinalysis, clinical chemistry or hematology; there was a non-significant increased absolute and relative liver weights that were not associated with histopathological lesions. NOAEL = 100,000 ppm (highest dose tested)	IUCLID/Occidental Chem Corp. 1992	Not specified as a guideline study, but follows general OECD guidelines.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		In a 28-day dermal exposure (5 day/week, on shaved abraded skin) study in rabbits, no significant treatment-related adverse effects were observed. No effects on body weights, urinalysis, hematology, clinical chemistry, gross pathology, or histopathology; a significant decrease in liver and ovary weights were reported in female rats, though there were no associated changes in absolute organ weights or histopathological effects. NOAEL = 2,000 mg/kg-day (highest dose tested)	IUCLID/Occidental Chem Corp. 1992	Not specified as a guideline study, but follows general OECD guidelines.
		Potential for repeated dose effects (Estimated by analogy and bioaccumulation).	Professional judgment	Estimated based on the high potential for bioaccumulation and by analogy to observations on decabromodiphenyl ether where adverse effects were not present in 90-day studies but were expressed following chronic exposure in a NTP study.
Skin Sensitization		**LOW: Bis(hexachlorocyclopentadieno) cyclooctane was not a skin sensitizer in one study of Guinea pigs.**		
	Skin Sensitization	Negative for skin sensitization, Guinea pigs	IUCLID/Brett, 1975	Not specified as a guideline study, but follows general OECD guidelines (modified Buehler).
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Eye Irritation		**VERY LOW: Bis(hexachlorocyclopentadieno) cyclooctane is not an eye-irritant in rabbits .**		
	Eye Irritation	Non-irritant, rabbit	IUCLID/Occidental Chem Corp., 1992	Not specified as a guideline study, but follows general OECD guidelines.
Dermal Irritation		**LOW: Estimated not to cause dermal irritation based on expert judgment.**		
	Dermal Irritation	Low potential for dermal irritation. (Estimated)	Expert judgment	Estimated based on expert judgment.
Endocrine Activity		**No data located.**		
				No data located.
Immunotoxicity		**No potential immunotoxic effects identified by expert judgment.**		
	Immune System Effects			No data located.
ECOTOXICITY				
ECOSAR Class		Vinyl/allyl halides		
Acute Toxicity		**LOW: Estimated data suggest no effects at saturation (NES) for the acute aquatic toxicity endpoints; experimental study details provided are insufficient to assess the hazard of acute aquatic toxicity, but are consistent with this hazard call.**		
Fish LC_{50}		*Lepomis macrochirus* (bluegill) 96-hour $TL_{50} \geq 100$ mg/L - highest dose tested (flow-through conditions)	IUCLID, 2003	Sufficient details were not available to assess the quality of this study (non- GLP, study was given a Klimish code of 3 - invalid).
		Lepomis macrochirus (bluegill) 96-hour $TL_{50} \geq 100$ mg/L - highest dose tested (static conditions)	IUCLID, 2003	Sufficient details were not available to assess the quality of this study (non-GLP, study was given a Klimish code of 3 - invalid).
		Fish 96-hour $LC_{50} = 1.89 \times 10^{-6}$ mg/L (Estimated) ECOSAR: vinyl/allyl halides	EPI	NES: The log K_{ow} of 11.27 for this chemical exceeds the SAR) limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
		Fish 96-hour $LC_{50} = 7.2 \times 10^{-6}$ mg/L (Estimated) ECOSAR: neutral organic	EPI	NES: The log K_{ow} of 11.27 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Daphnid LC_{50}	Daphnid 96-hour LC_{50} = $2.07x10^{-8}$ mg/L (Estimated) ECOSAR: vinyl/allyl halides	EPI	NES: The log K_{ow} of 11.27 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Daphnid 96-hour LC_{50} = $1.27x10^{-5}$ mg/L (Estimated) ECOSAR: neutral organics	EPI	NES: The log K_{ow} of 11.27 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
Green Algae Green Algae EC_{50}	Green algae 96-hour EC_{50} = $5.4x10^{-6}$ mg/L (Estimated) ECOSAR: vinyl/allyl halides	EPI	NES: The log K_{ow} of 11.27 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
	Green algae 96-hour EC_{50} = 0.00025 mg/L (Estimated) ECOSAR: neutral organics	EPI	NES: The log K_{ow} of 11.27 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
Chronic Aquatic Toxicity	**LOW: Estimated data suggest no effects at saturation (NES) for chronic aquatic toxicity endpoints.**		
Fish ChV	Fish 30-day ChV = $1.31x10^{-8}$ mg/L (Estimated) ECOSAR: vinyl/allyl halides	EPI	NES: The log K_{ow} of 11.27 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
	Fish 30-day ChV = $5.57x10^{-7}$ mg/L (Estimated) ECOSAR: neutral organics	EPI	NES: The log K_{ow} of 11.27 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
Daphnid ChV	Daphnid ChV = $6.06x10^{-6}$ mg/L (Estimated) ECOSAR: neutral organic	EPI	NES: The log K_{ow} of 11.27 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Green Algae ChV	Green algae ChV = $6.52x10^{-5}$ mg/L (Estimated) ECOSAR: vinyl/allyl halides	EPI	Chemical may not be soluble enough to measure this predicted effect; the toxicity value was determined from a predicted SAR using established acute-to-chronic ratios and ECOSAR regression techniques; NES: the log K_{ow} of 11.27 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
	Green algae ChV = 0.00049 mg/L (Estimated) ECOSAR: neutral organics	EPI	Chemical may not be soluble enough to measure this predicted effect; the toxicity value was determined from a predicted SAR using established acute-to-chronic ratios and ECOSAR egression techniques; NES: the log K_{ow} of 11.27 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
ENVIRONMENTAL FATE			
Transport	**Based on the Level III fugacity models incorporating the available experimental property data, bis(hexachlorocyclopentadieno) cyclooctane is expected to partition primarily to soil. Bis(hexachlorocyclopentadieno) cyclooctane is expected to be immobile in soil based on its estimated K_{oc}. Estimated volatilization half-lives indicate that it will be moderately volatile from surface water. Volatilization from dry surface is also not expected based on its estimated vapor pressure. In the atmosphere, bis(hexachlorocyclopentadieno) cyclooctane is expected to exist solely in the particulate phase, based on its estimated vapor pressure. Particulates may be removed from air by wet or dry deposition.**		
Henry's Law Constant (atm-m^3/mole)	$7.4x10^{-6}$ (Estimated)	EPI	

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	EPI; EPA, 2011b	Cutoff value for non mobile compounds according to SF assessment guidance.
		4,500,000 (Measured)	IUCLID, 2003 (citing from Chou et al., 1979)	Insufficient details were reported to assess the quality of this nonguideline study; however the results are consistent with other high MW, highly halogenated compounds.
	Level III Fugacity Model	Air ≤ 1% (Estimated) Water = 5% Soil = 92% Sediment = 3%	EPI	
Persistence		**VERY HIGH: The persistence concern for bis(hexachlorocyclopentadieno) cyclooctane is a result of experimental degradation studies and estimations based on quantitative structure-activity relationships (QSARs). Studies with aerobic and anaerobic sewage-sludge microorganisms reported no biodegradation in 2-3 to 6 weeks, respectively. Bis(hexachlorocyclopentadieno) cyclooctane has low water solubility and hydrolysis is not expected to be an important fate process; the two allylic chlorines capable of hydrolysis are at bridgehead locations which renders them resistant to displacement. Photolysis is not expected to be an important removal process with a measured degradation rate of <10% after 168 hours. Compiled, these degradation endpoints suggest a half-life >180 days. Environmental monitoring data supports a concern for very high persistence. Bis(hexachlorocyclopentadieno) cyclooctane has been detected in many places, including remote Arctic and Antarctic locations.**		
Water	**Aerobic Biodegradation**	0% degradation after 21 days; 0.001 and 100 mg/L bis(hexachlorocyclopentadieno) cyclooctane dilutions made in water inoculated with 2 ml/L settled sewage-sludge containing microorganisms (Measured)	IUCLID, 2003; Occidental Chemical Company, 2009	Adequate, nonguideline study.
		0% after 14 days; not readily biodegradable (Measured)	IUCLID, 2003; Occidental Chemical Company, 2009	Adequate, nonguideline study.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Volatilization Half-life for Model River	8 days (Estimated)	EPI	
	Volatilization Half-life for Model Lake	100 days (Estimated)	EPI	
Soil	**Aerobic Biodegradation**	<1% degradation after 2 weeks; OECD 301C measuring BOD; 100 ppm bis(hexachlorocyclopentadieno) cyclooctane with 30 ppm activated sludge inoculum (Measured)	MITI, 1998	Adequate, guideline study.
	Anaerobic Biodegradation	Not probable (Anaerobic-methanogenic biodegradation probability model)	EPI	
		0% after 2-6 weeks; Using C-14 labeled bis(hexachlorocyclopentadieno) cyclooctane; with anaerobic sewage sludge inoculum (Measured)	IUCLID, 2003; Occidental Chemical Company, 2009	Nonguideline study; sufficient details were not available to assess the quality of this study.
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	5.6 hours (Estimated)	EPI	
Reactivity	**Photolysis**	Half-life: >24 years (Measured) Reported as <10% after 168 hours	IUCLID, 2003	Adequate; nonguideline study.
	Hydrolysis	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to hydrolyze readily under environmental conditions.
Environmental Half-life		>180 days (Estimated)	EPI; PBT Profiler	Half-life estimated for the predominant compartment, as determined by EPI and the PBT Profiler methodology.

Bis(hexachlorocyclopentadieno) Cyclooctane CASRN 13560-89-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Bioaccumulation		**HIGH: Estimated BAF and available monitoring data suggest very high potential for bis(hexachlorocyclopentadieno) cyclooctane bioaccumulation.**		
	Fish BCF	23 to 121 (carp) (Measured); 14 to 96 (bluegill) (Measured)	MITI, 1998	Guideline study measured at a water solubility of 0.0027 mg/L.
		1.97 at 96 hours to 7.02 at 48 hours *Lepomis macrochirus* (Measured)	IUCLID, 2003	Nonguideline study.
	BAF	23,000 (Estimated)	EPI	
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		Bis(hexachlorocyclopentadieno) cyclooctane was detected in the particulate phase of air samples at 6 locations in the Great Lakes region; in Lake Erie and Lake Michigan sediment (Hoh et al., 2006); in Japanese industrial zones along the Pacific coast (Kubota, 1979); in Ottawa, Canada residential indoor dust samples (Zhu et al., 2007); in indoor dust collected from an e-waste recycling area and two control areas (rural and urban) in South China (Zheng et al., 2010); in atmosphere and seawater samples taken from East Greenland Sea and the northern and southern Atlantic, toward Antarctica (Moller et al., 2010, 2011).		
Ecological Biomonitoring		Bis(hexachlorocyclopentadieno) cyclooctane has been detected in archived fish (walleye) samples from Lake Erie (Hoh et al., 2006); fish from Lake Winnipeg and Lake Ontario food webs; five different fish species in South Korea; and plasma of nestling bald eagles (Sverko et al., 2011 citing Tomy, 2007; Kang, 2009 and Venier, 2010).		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011). Bis(hexachlorocyclopentadieno) cyclooctane was measured in human hair and indoor dust collected from an e-waste recycling area and two control areas in South China (Zheng et al., 2010); it was detected in serum sample in Guiyu and Haojiang, respectively (Ren et al., 2009).		

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Bisphenol A Bis-(diphenyl phosphate), BAPP

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

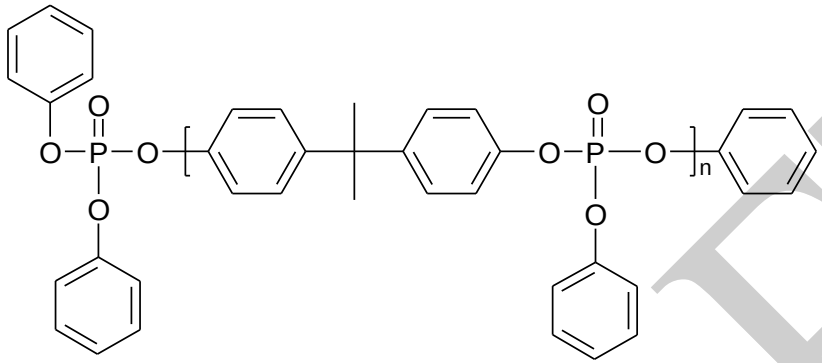
VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

§ Based on analogy to experimental data for a structurally similar compound.

◊ The highest hazard designation of a representative component of the oligomeric mixture with MWs <1,000.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Bisphenol A Bis-(diphenyl phosphate), BAPP	181028-79-5	L	*L*	L	*L*	*L*§	L	L	L		L	L	L	L	H	*H*◊

BAPP



CASRN: 181028-79-5

MW: 693(n = 1); >1,000 (n = 2)

MF: $C_{39}H_{34}O_8P_2$ (n = 1; CASRN 5945-33-5)

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: c1(C(C)(C)c2ccc(OP(=O)(Oc3ccccc3)Oc3ccccc3)cc2)ccc(OP(=O)(Oc2ccccc2)Oc2ccccc2)cc1 (n = 1; CASRN 5945-33-5)

Synonyms: Phosphoric trichloride, reaction products with bisphenol A and phenol (TSCA Inventory); Phosphoric acid, isopropylidenedi-p-phenylene tetraphenyl ester; 2,2-Bis[4-[bis(phenoxy)phosphoryloxy]phenyl]propane; 4,4'-(Isopropylidenediphenyl) bis(diphenyl phosphate); Bisphenol A bis(diphenyl phosphate); Bisphenol A tetraphenyl diphosphate; BADP; BDP; BPADP; Fyrolflex BDP
Phosphoric acid, P,P'-[(1-methylethylidene)di-4,1-phenylene] P,P,P',P'-tetraphenyl ester (TSCA Inventory) for 5945-33-5

Chemical Considerations: This alternative is a polymer. The oligomer where n = 1 (also referred to as CASRN 5945-33-5) has a MW <1,000 and is amenable to EPI v4.0 estimation methods for physical/chemical and environmental fate values in the absence of experimental data. In commerce, CASRN 5945-33-5 is used interchangeably with 181028-79-5 and both represent in practice a substance that is 80+% BAPP with higher homologues (n=1,2 or 3). The higher MW oligomers that have MWs >1,000 are assessed together using the Sustainable Futures (SF) polymer assessment criteria (U.S. EPA, 2010).

Polymeric: Yes **Oligomers:** The n = 1 structure comprises 85% of the mixture, with the balance primarily made up of higher oligomers (n = 2, 3, 4, etc.). The commercial mixture contains triphenyl phosphate as an impurity.	
Metabolites, Degradates and Transformation Products: None	
Analogs: Confidential compounds **Endpoint(s) using analog values:** Developmental effects	**Analog Structures:** No structure provided for confidential compounds.
Structural Alerts: None	
Risk Phrases: For CASRN 5945-33-5 R53- May cause long-term adverse effects in the aquatic environment (ESIS, 2012).	
Hazard and Risk Assessments: Risk assessment completed for BAPP by the National Industrial Chemicals Notification and Assessment Scheme (NICNAS NA/869, 2000; NICNAS NA/773, 2000).	
U.S. EPA TSCA Regulatory Status: 181028-79-5 was a commenced Premanufacture Notice submission. Both chemicals (181028-79-5 and 5945-33-5) are listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory**.**	

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	41.3-68.6 (Measured)	Hogg, 1997; NICNAS NA/773, 2000	Results from DSC analysis were originally reported as a boiling point range of 41.3-68.6°C in the NICNAS document. The melting point range is likely from a commercial product or mixture.
	7 (Measured OECD 102)	Chemtura, 2011	Reported for oligomer where n=1 CASRN 5945-33-5.
Boiling Point (°C)	>201 (decomposes) (Measured)	Hogg, 1997	Reported to decompose without boiling at temperatures above 201°C.
	>240 – 250 (Measured)	Lightbody, 1999	Inadequate; the reported data are for a commercial mixture.
	Decomposes above 350 without boiling (OECD 103)	Chemtura, 2011	Reported for oligomer where n=1 CASRN 5945-33-5.
Vapor Pressure (mm Hg)	$<9x10^{-6}$ at 25°C (Extrapolated)	Tremain, 1997	Although a definitive value could not be reported in this study, the test chemical contained 1-3% triphenyl phosphate and residual phenol, which may have contributed to scatter in the data. These results suggest, however, that the EPI estimates for this endpoint are reasonable.
	$2.1x10^{-8}$ (Estimated, n = 1)	EPI; EPA, 2010	Although the higher MW oligomers are outside the domain of the available estimation methods, their vapor pressures are anticipated to be below the cutoff values according to SF assessment guidance.

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	$2.3x10^{-18}$ at 25°C (Extrapolated)	Tremain, 2000; EPA, 2010	Inadequate; the data are for the commercial mixture extrapolated to 25°C. However, the data are consistent with a vapor pressure below the cutoff values for the higher MW oligomers according to SF assessment guidance.
	$1x10^{-6}$ (Measured OECD 104)	Chemtura, 2011	Reported for oligomer where n=1 CASRN 5945-33-5.
Water Solubility (mg/L)	0.389 – 0.462 (Measured)	Hogg, 1997	Although the commercial mixture was likely used as test material, the reported value provides an upper boundary for the most soluble component of the mixture, the oligomer with n = 1. The experiment was performed in acidic conditions (pH 5.5-6) and the purity of the test chemical was not specified.
	$<10^{-3}$ (Estimated)	EPI; EPA, 2010	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture. Although the higher MW oligomers are outside the domain of the available estimation methods, their water solubilities are anticipated to be below the cutoff values according to SF assessment guidance.
	$<2x10^{-2}$ (Measured)	Lightbody, 1999	Inadequate; the reported data are for a commercial mixture.

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Log K_{ow}	>6 (Measured)	Iwami, 1995	The commercial mixture was likely used as test material; cutoff too low to address endpoints for the hazard assessment.
	>10 (Estimated)	EPI; EPA, 2010	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture. Although the higher MW oligomers are outside the domain of the available estimation methods, their K_{ow} values are anticipated to be above the cutoff values.
	4.0 (n = 1); 5.2 (n = 2) (Measured)	Lightbody, 1999	Inadequate; the reported data are for a commercial mixture. The results are more consistent with the measured value for the triphenyl phosphate impurity (log K_{ow}=4.59) than with the BAPP oligomers.
	4.5, >4.9 (Measured OECD 107)	Chemtura, 2011	Reported for oligomer where n=1 CASRN 5945-33-5.
Flammability (Flash Point)	>300 (Measured)	NICNAS NA/773, 2000	Reported in a secondary source, study details and test conditions were not provided.
	>360, closed cup (Measured)	NICNAS NA/869, 2000	
	281 (Measured EEC method No A9)	Chemtura, 2011	Reported for oligomer where n=1 CASRN 5945-33-5.
Explosivity	Not explosive (Measured to EEC method No A14)	Chemtura, 2011	Reported for oligomer where n=1 CASRN 5945-33-5.
Pyrolysis			No data located.

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
pH		Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a		Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Based on professional judgment, absorption is not expected for any route of exposure for the neat material. Poor absorption of the low MW fraction in solution can be expected in all routes.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No absorption is expected for any route of exposure; poor absorption of low MW fraction (0% <500, 85% <1,000) in solution by all routes (Estimated by analogy)	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/chemical properties.
Acute Mammalian Toxicity		**LOW: Based on oral and dermal LD_{50} values of >2,000 mg/kg in rats for both the commercial mixture and its predominant component. No data located regarding the acute inhalation hazard.**		
Acute Lethality	**Oral**	Rat oral LD_{50} >2,000 mg/kg	NICNAS NA/869, 2000	Reported in a secondary source. Study conducted according to OECD guidelines (OECD 401). Data are for commercial mixture.
		Rat oral LD_{50} >2,000 mg/kg	NICNAS NA/773, 2000	Reported in a secondary source. Study conducted according to EEC/OECD guidelines (OECD 401). Data are for the predominant component.
	Dermal	Rat dermal LD_{50} >2,000 mg/kg	NICNAS NA/869, 2000	Reported in a secondary source. Study conducted according to EEC/OECD guidelines (OECD 402). Data are for commercial mixture.

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Rat dermal LD_{50} >2,000 mg/kg	NICNAS NA/773, 2000	Reported in a secondary source. Study conducted according to EEC/OECD guidelines (OECD 402). Data are for the predominant component.
	Inhalation			No data located.
Carcinogenicity		**LOW: Estimated to have low potential for carcinogenicity based on expert judgment. No data located.**		
	OncoLogic Results			No data located; not amenable to available estimation methods.
	Carcinogenicity (Rat and Mouse)	Low potential for carcinogenicity. (Estimated)	Expert judgment	Estimated based on expert judgment.
	Combined Chronic Toxicity/ Carcinogenicity			
Genotoxicity		**LOW: There is uncertain potential for mutagenicity based on experimental studies. Neither the commercial mixture nor the predominant component induced gene mutations in several *in vitro* assays in bacteria and did not induce chromosomal aberrations in CHO or CHL cells *in vitro*. The commercial mixture did not increase micronucleated polychromatic erythrocytes in mouse bone marrow cells *in vivo*.**		
	Gene Mutation *in vitro*	Negative, Ames assay (standard plate) in *Salmonella typhimurium* strains TA98, TA100, TA1537, TA1535, and *E. coli* WP2uvrA with and without metabolic activation	NICNAS NA/869, 2000	Sufficient study details were reported in a secondary source; used OECD test guidelines (OECD 471 & 472). Data are for commercial mixture.
		Negative, Ames assay (standard plate) in *Salmonella typhimurium* strains TA98, TA100, TA1537, TA1535, and *E. coli* WP2uvrA with and without metabolic activation	NICNAS NA/773, 2000	Sufficient study details were reported in a secondary source; used OECD test guidelines (OECD 471 & 472). Data are for the predominant component.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	Uncertain potential for mutagenicity based on a positive result for chromosome aberrations in CHL cells (Estimated by analogy)	Professional judgment	Based on a structurally similar confidential analog.

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Negative, did not produce chromosomal aberrations in CHO cells with and without metabolic activation	NICNAS NA/869, 2000	Sufficient study details were reported in a secondary source; used OECD test guidelines (OECD 473). Data are for commercial mixture.
		Negative, did not produce chromosomal aberrations in CHL cells with and without metabolic activation	NICNAS NA/773, 2000	Sufficient study details were reported in a secondary source; used EC/EEC test guidelines (EC Directives 87/18/EEC and 88/320/EEC). Data are for the predominant component.
	Chromosomal Aberrations *in vivo*	Negative; did not increase micronucleated polychromatic erythrocytes in bone marrow cells of mice treated with 2,000 mg/kg at 0 and 24 hours. No mortalities or adverse effects were observed in treated animals.	NICNAS NA/869, 2000	Sufficient study details were reported in a secondary source; used OECD test guidelines (OECD 474). Data are for commercial mixture.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: Estimated to have low potential for reproductive effects based on expert judgment. No data located.**		
	Reproduction/ Developmental Toxicity Screen	Low potential for reproductive effects. (Estimated)	Expert judgment	Estimated based on expert judgment.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**LOW: Estimated to have low potential for developmental effects based on a structurally similar confidential analog. No fetal effects reported. Experimental data located are inadequate to designate a hazard concern for this endpoint.**		
	Reproduction/ Developmental Toxicity Screen	Oral, developmental study; no fetal effects reported. (Estimated by analogy)	Professional judgment	Based on a structurally similar confidential analog.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Prenatal Development	14-day developmental study in rats via oral gavage NOAEL: 1,000 mg/kg-day	Illinois EPA, 2007; WA Department of Health, 2006	Insufficient study details reported in a secondary source. Data are for commercial mixture.
	Postnatal Development			No data located.
Neurotoxicity		**LOW: There were no neurotoxic effects observed at doses up to 1,000 mg/kg-day following 28-day oral administration of the commercial mixture to rats.**		
	Neurotoxicity Screening Battery (Adult)			
		In a 28-day oral (gavage) study of Sprague-Dawley rats, there were no treatment-related changes in any of the parameters measured (body weight gain, food consumption, clinical signs, neurotoxicology parameters, organ weights, clinical chemistry, hematology, gross necropsy, histopathology) NOEL ≥1,000 mg/kg-day (highest dose tested)	NICNAS NA/869, 2000; Washington Department of Health, 2006	Sufficient study details were reported; used OECD test guidelines (OECD 407). Data are for commercial mixture.

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects		**LOW: There were no treatment-related changes in systemic toxicity parameters measured at doses up to 1,000 mg/kg-day in a 28-day oral study in Sprague-Dawley rats. Although only one species has been studied, these were comprehensive OECD or EEC guideline studies that found no dose-related effects for either the commercial mixture or its predominant component.**		
		In a 28-day oral (gavage) study in Sprague-Dawley rats, there were no treatment-related changes in any of the parameters measured (body weight gain, food consumption, clinical signs, neurotoxicology parameters, organ weights, clinical chemistry, hematology, gross necropsy, histopathology) NOEL ≥1,000 mg/kg-day (highest dose tested)	NICNAS NA/869, 2000	Sufficient study details were reported; used OECD test guidelines (OECD 407). Data are for commercial mixture.
		In a 28-day oral (gavage) study in Sprague-Dawley rats, there were no treatment-related changes in any of the parameters measured (clinical signs, organ weights, clinical chemistry, hematology, gross necropsy, histopathology) NOEL ≥1,000 mg/kg-day (highest dose tested)	NICNAS NA/773, 2000	Sufficient study details were reported; used EEC test guidelines (EEC Directive 92/69/EEC, Method B7). Data are for the predominant component.
Skin Sensitization		**LOW: Commercial mixture and its predominant component were not skin sensitizers in two studies of guinea pigs.**		
	Skin Sensitization	Non-sensitizing, guinea pig	NICNAS NA/869, 2000	Conducted according to EEC/OECD guidelines (OECD 406). Data are for commercial mixture.
		Non-sensitizing, guinea pig	NICNAS NA/773, 2000	Conducted according to EEC/OECD guidelines (OECD 406). Data are for the predominant component.

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Commercial mixture was slightly irritating and predominant component was non-irritating to rabbit skin.**		
	Eye Irritation	Slightly irritating, rabbit	NICNAS NA/869, 2000	Conducted according to EEC/OECD guidelines (OECD 405). Data are for commercial mixture.
		Non-irritant, rabbit	NICNAS NA/773, 2000	Conducted according to EEC/OECD guidelines (OECD 405). Data are for the predominant component.
Dermal Irritation		**LOW: Commercial mixture was slightly irritating and predominant component was non-irritating to rabbit skin.**		
	Dermal Irritation	Slightly irritating, rabbit	NICNAS NA/869, 2000	Conducted according to EEC/OECD guidelines (OECD 404). Data are for commercial mixture.
		Non-irritant, rabbit	NICNAS NA/773, 2000	Conducted according to EEC/OECD guidelines (OECD 404). Data are for the predominant component.
Endocrine Activity		**BAPP is not expected to affect endocrine activity based on expert judgment. BAPP does not release bisphenol A. No data located.**		
		Low potential for endocrine activity. (Estimated)	Expert judgment	Estimated based on expert judgment.
Immunotoxicity		**Estimated to have low potential for immunotoxicity based on expert judgment. No data located.**		
	Immune System Effects	Low potential for immunotoxicity. (Estimated)	Expert judgment	Estimated based on expert judgment.
ECOTOXICITY				
ECOSAR Class		Esters, Esters (phosphate)		

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Acute Toxicity	**LOW: Experimental data for both the predominant component (n = 1) and the commercial mixture for fish, daphnia, and algae indicate no effects up to the limits of the water solubility.**		
Fish LC_{50}	*Oncorhynchus mykiss* (rainbow trout), 96-hour LC_{50} > 0.025 mg/L NOEC = 0.025 mg/L	NICNAS NA/869, 2000	Conducted according to OECD guidelines (OECD 203); not toxic up to the limits of its water solubility.
	Oncorhynchus mykiss (rainbow trout), 96-hour LC_{50} >1 mg/L NOEC >1 mg/L (Experimental)	NICNAS NA/773, 2000	Conducted according to OECD guidelines (OECD 203); not toxic up to the limits of its water solubility. Data are for the predominant component.
Daphnid LC_{50}	*Daphnia magna*, 48-hour EC_{50} >0.034 mg/L; NOEC = 0.034 mg/L (immobilization) (Experimental)	NICNAS NA/869, 2000	Conducted according to OECD guidelines (OECD 202); not toxic up to the limits of its water solubility. Data are for commercial mixture.
	Daphnia magna, 48-hour EC_{50} >1 mg/L; NOEC >1 mg/L (immobilization) (Experimental)	NICNAS NA/773, 2000	Conducted according to OECD guidelines (OECD 202); not toxic up to the limits of its water solubility. Data are for the predominant component.
Green Algae EC_{50}	*Selanastrum subspicatus* 72-hour EbC_{50} >0.02 mg/L; NOEC = 0.02 mg/L (growth) (Experimental)	NICNAS NA/869, 2000	Conducted according to OECD guidelines (OECD 201); not toxic up to the limits of its water solubility. Data are for commercial mixture.
	Selanastrum subspicatus 72-hour EbC_{50} >1 mg/L; NOEC >1 mg/L (growth) (Experimental)	NICNAS NA/773, 2000	Conducted according to OECD guidelines (OECD 201); not toxic up to the limits of its water solubility. Data are for the predominant component.
Chronic Aquatic Toxicity	**LOW: Experimental data for the commercial mixture in *Daphnia* indicate no toxicity effects up to the limits of the water solubility. Estimates for fish and algae also suggest no effects at saturation (NES).**		

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Fish ChV	Fish ChV = NES (Estimated) ECOSAR: neutral organic	EPI	Estimated data based on the high K_{ow} of the predominant oligomer component, n = 1, representing 85% of the commercial mixture. Although the higher MW oligomers are outside the domain of the estimation method, they are also anticipated to display NES.
Daphnid ChV	*Daphnia magna*, 21-day EC_{50} >0.02 mg/L; NOEC = 0.02 mg/L (reproduction test) (Experimental)	NICNAS NA/869, 2000	Conducted according to OECD guidelines (OECD 211); not toxic up to the limits of its water solubility. Data are for commercial mixture.
Saltwater Invertebrate ChV			No data located.
Green Algae ChV	Green algae ChV = NES (Estimated) ECOSAR: esters, esters (phosphate), and neutral organic	EPI	Estimated data based on the high K_{ow} of the predominant oligomer component, n = 1, representing 85% of the commercial mixture. Although the higher MW oligomers are outside the domain of the estimation method, they are also anticipated to display NES.
ENVIRONMENTAL FATE			
Transport	**The environmental fate is described using estimates on the lowest MW oligomer of BAPP, which is the predominant component. Based on the Level III fugacity models incorporating the available experimental property data, the lowest MW oligomer is expected to partition primarily to soil and sediment. BAPP is expected to be immobile in soil based on its estimated K_{oc}. Leaching of BAPP through soil to groundwater is not expected to be an important transport mechanism. Estimated volatilization half-lives indicate that BAPP will be nonvolatile from surface water. Volatilization from dry surface is also not expected based on its vapor pressure. In the atmosphere, BAPP is expected to exist solely in the particulate phase, based on its estimated vapor pressure. Particulates may be removed from air by wet or dry deposition. The higher MW components of the commercial mixture are anticipated to behave similarly to that described above.**		

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Henry's Law Constant (atm-m^3/mole)	**Predominant component (5945-33-5):** $<10^{-8}$ (Estimated)	EPI; Professional judgment	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture. The higher MW oligomers are also expected to have Henry's Law Constant values below this cutoff.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	$>3.39x10^4$ (Measured)	Hogg, 1997	Data obtained using an HPLC method similar to OECD TGP/94.75 method. Although a commercial mixture was likely used as test material, the reported value provides a lower boundary for the most mobile component of the mixture, the oligomer with n = 1.
		Predominant component (5945-33-5): 30,000 (Estimated)	EPI	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture.
	Level III Fugacity Model	Air = <1% (Estimated) Water = 1.1% Soil = 42% Sediment = 57%	EPI	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture.
Persistence		**HIGH: Experimental studies on the commercial mixture, which is estimated to contain approximately 85% BAPP, determined BAPP to be not readily biodegradable by a MITI-I (OECD TG 301C) test as 6% biodegradation occurred over 28 days in sewage sludge. BAPP is not expected to undergo hydrolysis and therefore not release bisphenol A at appreciable rates, as it does not contain functional groups that readily hydrolyze. The hydrolysis half-life of the commercial mixture was >1 year at pH 5 to 9. BAPP does not contain chromophores that absorb at wavelengths >290 nm, and therefore is not expected to be susceptible to direct photolysis by sunlight. The atmospheric half-life of BAPP is estimated to be 5.5 hours, although it is expected to exist primarily in the particulate phase in air.**		

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Water	**Aerobic Biodegradation**	Days-weeks (Primary survey model) Months (Ultimate survey model)	EPI	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture.
		6% biodegradation detected after 28 days in activated sludge according to a MITI-I Ready Test (OECD TG 301C) (Measured)	Iwami, 1994	The commercial mixture was likely used as test material.
		2% biodegradation detected after 28 days in sewage sludge according to Ready Test Modified Sturm Test (OECD TG 301). (Measured)	Armstrong and White, 1999	The data are for the commercial mixture.
	Volatilization Half-life for Model River	>1 year (Estimated)	EPI	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	EPI	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture.
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation	Not probable (Anaerobic-methanogenic biodegradation probability model)	EPI	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Air	**Atmospheric Half-life**	5.5 hours (Estimated)	EPI	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
	Hydrolysis	At 25°C, >1 year at pH 4.0, 7.0 and 9.0 (Measured)	Hogg, 1997	The commercial mixture was likely used as test material. Data indicate the resistance of the material to hydrolysis under environmental conditions. Purity of the test chemical was not specified.
Environmental Half-Life		>1 year (Estimated)	EPI; PBT Profiler	Half-life estimated for the predominant compartment, as determined by EPI and the PBT Profiler methodology for the predominant oligomer component, n = 1, representing 85% of the commercial mixture.
Bioaccumulation		**HIGH: The estimated BAF of 1,100 for the predominant component of the mixture, the only oligomer with a MW <1,000, suggests that BAPP may bioaccumulate in higher trophic levels.**		
	Fish BCF	BCF range: <= 1.1 - <= 159 BCF range: 6.8 – 62 (Estimated by analogy)	Chemtura, 2011	Reported for oligomer where n=1 CASRN 5945-33-5.
		66 (Estimated)	EPI	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture.

Bisphenol A Bis-(diphenyl phosphate) CASRN 181028-79-5 and 5945-33-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	BAF	1,100 (Estimated)	EPI	Estimated data based on the predominant oligomer component, n = 1, representing 85% of the commercial mixture.
	Metabolism in fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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Brominated Epoxy Resin End-Capped with Tribromophenol

Screening Level Hazard Summary

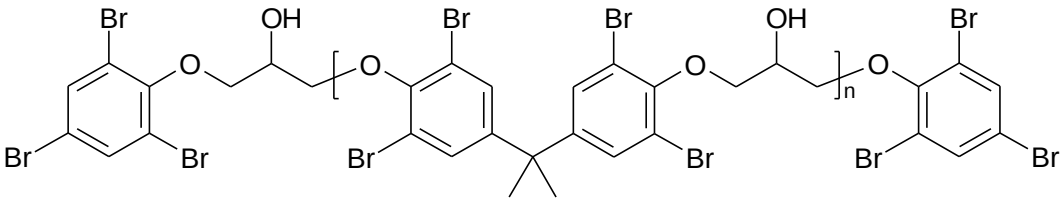
This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

[d] This hazard designation is driven by potential for lung overloading as a result of dust forming operations.

Chemical	CASRN	Human Health Effects										Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Brominated Epoxy Resin End-Capped with Tribromophenol	135229-48-0	***L***	***L***	**L**	***L***	***L***	***L***	***M***[d]	**L**		**L**	**VL**	***L***	***L***	***VH***	***L***

Brominated Epoxy Resin End-Capped with Tribromophenol



CASRN: 135229-48-0

MW: 15,000; 0%< 1,000

MF: $(C_{15}H_{12}Br_4O_2 \cdot C_6H_3Br_3O \cdot C_3H_5ClO)_n$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: This polymer with MW >1,000 and no low MW components is not amenable to SMILES notation.

Synonyms: 2,2'-[(1-Methylethylidene)bis[(2,6-dibromo-4,1-phenylene)oxymethylene]]bisoxirane polymer with 2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol and 2,4,6-tribromophenol; Phenol, 4,4'-(1-methylethylidene)bis[2,6-dibromo-, polymer with (chloromethyl)oxirane and 2,4,6-tribromophenol

Chemical Considerations: This alternative is a polymer. The extent of polymerization and thus average MW is formulation dependent. The higher MW oligomers with a MW >1,000 are assessed together using the Sustainable Futures (SF) polymer assessment criteria (U.S. EPA, 2010). Additionally, lower MW formulations of brominated epoxy resin end-capped with tribromophenol exist and the simplest oligomer, comprised of each monomer, has a MW of 970. Although below the cutoff of 1,000 used in the polymer assessment criteria, this oligomer is anticipated to possess physical/chemical properties similar to that of the higher MW material, including limited absorption in biological systems. As a result, the assessment of the oligomers with a MW <1,000 will be performed in a manner identical to the remaining components of the polymer.

Polymeric: Yes
Oligomers: This substance is a brominated epoxy polymer end-capped with tribromophenol. Tribromophenol end-capped epoxy polymer typically consists of oligomers with an average MW of 15,000 with 0% MW <1,000.The MW of the simplest oligomer comprised of each monomer is 970.

Metabolites, Degradates and Transformation Products: None

Analog: No analog
Endpoint(s) using analog values: Not applicable

Analog Structure: Not applicable

Structural Alerts: None identified

Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).

Hazard and Risk Assessments: A Hazard Characterization was completed for Brominated epoxy resin end-capped with tribromophenol in 2010 (U.S. EPA, 2010)

U.S. EPA TSCA Regulatory Status: Listed on the TSCA Chemical Inventory as EPA Acc. No. 153958 CASRN 534584-61-7 (ICL Industrial Products, 2009). This chemical is not listed on the non-confidential TSCA Inventory.

Brominated Epoxy Resin End-Capped with Tribromophenol CASRN 135229-48-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	180–220 (Measured)	ICL Industrial Products, 2009	The melting points reported cover a broad range and are anticipated to be formulation specific liquid-glass transition temperatures for the commercial product F-3100
	105–120 (Measured)	NICNAS, 2006	The melting points reported cover a broad range and are anticipated to be formulation specific liquid-glass transition temperatures for the commercial product F-3020, the brominated epoxy resin end-capped with tribromophenol with low MW oligomers that is expected to behave similarly to the high MW polymer.
Boiling Point (°C)	>300 (Estimated)	Professional judgment	Cutoff value used for large, high MW non-ionic polymers.
	Decomposition temperature: 340 (Measured)	ICL Industrial Products, 2009	The melting points reported cover a broad range and are anticipated to be formulation specific liquid-glass transition temperatures for the commercial product F-3100.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW non-ionic polymers according to SF polymer assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for non-ionic polymers according to SF polymer assessment guidance.

Brominated Epoxy Resin End-Capped with Tribromophenol CASRN 135229-48-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Log K_{ow}			No data located; polymers with a MW >1,000 are outside the domain of the available estimation methods.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.

Brominated Epoxy Resin End-Capped with Tribromophenol CASRN 135229-48-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**There is no absorption expected for any route of exposure. This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No absorption is expected for all routes of exposure (Estimated)	Professional judgment	Estimated based on limited bioavailability and professional judgment.
Acute Mammalian Toxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is of low potential for acute mammalian toxicity.**		
	Oral	Rat Oral LD_{50} >2,000 mg/kg (Acute Oral Toxicity-Limit Test).	NICNAS, 2006	Reported in a secondary source. Conducted according to OECD TG 401 guideline study for the commercial product F-3020, the brominated epoxy resin end-capped with tribromophenol with low MW oligomers that is expected to behave similarly to the high MW polymer.
	Dermal			No data located.
	Inhalation	This polymer's MW_n is >10,000; potential for irreversible lung damage as a result of lung overloading (Estimated)	Professional judgment**;** EPA, 2011	Based on SF polymer assessment guidance.
Carcinogenicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have few to no residual monomers, crosslinking, swellability, dispersability, reactive functional groups, potential for inhalation nor hindered amine groups and therefore has low potential for carcinogenicity.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Chronic Toxicity/ Carcinogenicity			

Brominated Epoxy Resin End-Capped with Tribromophenol CASRN 135229-48-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Genotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for genotoxicity. Bacterial reverse mutation test is negative for gene mutations.**		
	Gene Mutation *in vitro*	Negative for gene mutations in *Salmonella typhimurium* strains TA1535, TA1537, TA1538, TA100, TA98 with and without exogenous metabolic activation	NICNAS, 2006	Reported in secondary sources. Guideline study according to OECD TG 471 for the commercial product F-3020, the brominated epoxy resin end-capped with tribromophenol with low MW oligomers that is expected to behave similarly to the high MW polymer.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*			No data located.
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for reproductive effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			

Brominated Epoxy Resin End-Capped with Tribromophenol CASRN 135229-48-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for developmental effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			
	Postnatal Development			
Neurotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for neurotoxicity.**		
	Neurotoxicity Screening Battery (Adult)			No data located.
Repeated Dose Effects		**MODERATE: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability; however, because the MW_n is >10,000 there is the possibility of lung overloading in dust forming conditions.**		
		This polymer MW_n is >10,000; potential for irreversible lung damage as a result of lung overloading (Estimated)	Professional judgment**;** EPA, 2011	Based on SF polymer assessment guidance.
Skin Sensitization		**LOW: No evidence of reactions indicative of skin sensitization to brominated epoxy resin end-capped with tribromophenol in a study of guinea pigs.**		
	Skin Sensitization	No evidence of reactions indicative of skin sensitization, guinea pig skin sensitization – Magnusson & Kligman maximization test.	NICNAS, 2006	Reported in a secondary source. Conducted according to OECD TG 406 guideline study for the commercial product F-3020, the brominated epoxy resin end-capped with tribromophenol with low MW oligomers that is expected to behave similarly to the high MW polymer.

Brominated Epoxy Resin End-Capped with Tribromophenol CASRN 135229-48-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Brominated epoxy resin end-capped with tribromophenol is a mild eye irritant in rabbits; irritation begins to clear within 24 hours and is completely cleared within 48 hours.**		
	Eye Irritation	Minimally irritating, rabbit clearing within 24 hours acute eye irritation/corrosion.	NICNAS, 2006	Reported in a secondary source. Conducted according to OECD TG 405 guideline study for the commercial product F-3020, the brominated epoxy resin end-capped with tribromophenol with low MW oligomers that is expected to behave similarly to the high MW polymer.
Dermal Irritation		**VERY LOW: Brominated epoxy resin end-capped with tribromophenol is not irritating to the skin of rabbits.**		
	Dermal Irritation	Non-irritating to the skin of rabbits, acute dermal irritation/corrosion study.	NICNAS, 2006	Reported in a secondary source. Conducted according to OECD TG 404 guideline study for the commercial product F-3020, the brominated epoxy resin end-capped with tribromophenol with low MW oligomers that is expected to behave similarly to the high MW polymer.
Endocrine Activity		**This polymer is large, with a MW >1,000. It is not expected to have endocrine activity due to its poor bioavailability and inability to be readily metabolized in the body.**		
		Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.

Brominated Epoxy Resin End-Capped with Tribromophenol CASRN 135229-48-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Immunotoxicity		**This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is of low potential for immunotoxicity.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**LOW: Non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to display no effects at saturation (NES). These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for acute toxicity for those materials that display NES.**		
Fish LC_{50}		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will NES.
Daphnid LC_{50}		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity		**LOW: Non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to display NES. These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for chronic aquatic toxicity for those materials that display NES.**		
Fish ChV		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.

Brominated Epoxy Resin End-Capped with Tribromophenol CASRN 135229-48-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Daphnid ChV		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae ChV		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that this polymer is anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of <10^{-8} atm-m^3/mole indicates that it is not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that it is not anticipated to migrate from soil into groundwater and also has the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	<10^{-8} (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to have low vapor pressure and are not expected to undergo volatilization according to polymer assessment guidance.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000(Estimated)	Professional judgment; EPA, 2010	Cutoff value used for large, high MW polymers. High MW polymers are expected to absorb strongly to soil and sediment according to polymer assessment guidance.
	Level III Fugacity Model			No data located.
Persistence		**VERY HIGH: This polymer is large, with a MW >1,000. It is expected to have negligible water solubility and poor bioavailability to microorganisms indicating that neither biodegradation nor hydrolysis are expected to be important removal processes in the environment. Although debromination by photodegradation of polybrominated benzenes has been observed, this process is not anticipated to lead to ultimate removal of the material. As a result, a half-life for this high MW polymer of >180 days leads to a potential for very high persistence.**		

Brominated Epoxy Resin End-Capped with Tribromophenol CASRN 135229-48-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW polymers according to SF polymer assessment guidance.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation			No data located.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Professional judgment	Bromine substituents are susceptible to photolysis however; this is expected to be a relatively slow process for brominated epoxy resin end-capped with tribromophenol and is not anticipated to lead to ultimate removal of the material.
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.

Brominated Epoxy Resin End-Capped with Tribromophenol CASRN 135229-48-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Environmental Half-Life		>180 days (Estimated)	Professional judgment	The substance has a MW >1,000 and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. Other degradative processes under environmental conditions are not anticipated to be facile.
Bioaccumulation		**LOW: Due to the large size and water insolubility of this high MW polymer, it is of low potential for bioconcentration or bioaccumulation.**		
	Fish BCF	<100 (Estimated)	Professional judgment	Cutoff value for large, high MW, insoluble polymers according to SF polymer assessment guidance.
	BAF			No data located.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

CDC (Centers for Disease Control and Prevention). *Fourth national report on human exposure to environmental chemicals, updated tables*. Department of Health and Human Services. **2011.** http://www.cdc.gov/exposurereport/pdf/Updated_Tables.pdf (accessed on May 10, 2011).

[SF Assessment Guidance] EPA (Environmental Protection Agency). Sustainable Futures Summary Assessment. *Assessment of Discrete Organic Chemicals.* U.S. Environmental Protection Agency: Washington D.C. **2011**. http://www.epa.gov/oppt/sf/pubs/iad_discretes_092011.pdf

U.S. EPA (Environmental Protection Agency). Office of Pollution Prevention and Toxics. *Screening-Level Hazard Characterization Document for Phosphoryl Chloride, Polymer with Resorcinol Phenyl Ester (CASRN 125997-21-9).* Environmental Protection Agency: Washington D.C. http://www.epa.gov/opptintr/sf/pubs/noncan-screen.htm#systemic (accessed February 09, **2011**).

EPA (Environmental Protection Agency). Sustainable Futures. *Using NonCancer Screening within the SF Initiative.* Environmental Protection Agency: Washington D.C. **2010**. http://www.epa.gov/chemrtk/hpvis/hazchar/125997219_Phosphoryl%20chloride,%20polymer%20with%20resorcinol%20phenyl%20ester_%20June%202010.pdf (accessed April 5, 2012).

ESIS (European chemical Substances Information System) Classification, labeling and packaging of dangerous substances annex VI to regulation (EC) No 1272/2008 [Online] available at: http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=cla as of May 10, **2011**.

ICL Industrial Products. Material Safety Data Sheet (MSDS) for *F-3100*. www.icl-ip.com. **2009**.

ICL Industrial Products. Material Safety Data Sheet (MSDS) for *F-3014*. www.icl-ip.com. **2010**.

NICNAS (National Industrial Chemicals Notification and Assessment Scheme). *Phenol, 4,4'-(1-methylethylidene)bis[2,6-dibromo-, polymer with (chloromethyl)oxirane and 2,4,6-tribromophenol (F-3020).* File No. LTD/1261. **2006.**

Brominated Polyacrylate

Screening Level Hazard Summary

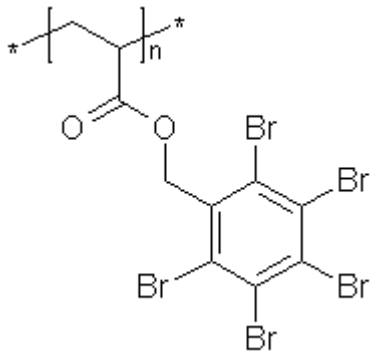
This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

[d] This hazard designation is driven by potential for lung overloading as a result of dust forming operations.

Chemical	CASRN	Human Health Effects										Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Brominated Polyacrylate	59447-57-3	*L*	*L*	*L*	*L*	*L*	*L*	*M* [d]	*L*		*L*	*L*	*L*	*L*	*VH*	*L*

Brominated Polyacrylate

<table>
<tr><td>  </td><td>CASRN 59447-57-3
MW: 80,000 (Measured); 0% <1,000
MF: $(C_{10}H_5Br_5O_2)_n$
Physical Forms:
Neat: Solid
Use: Flame retardant</td></tr>
<tr><td colspan="2">SMILES: This polymer with MW >1,000 and no low MW components is not amenable to SMILES notation.</td></tr>
<tr><td colspan="2">Synonyms: 2-Propenoic acid, (2,3,4,5,6-pentabromophenyl)methyl ester, homopolymer (TSCA Inventory); 2-Propenoic acid, (pentabromophenyl)methyl ester, homopolymer; Ameribrom FR 1025; FR 1025; FR 1025P; PBB-PA; Pentabromo-benzyl-acrylate, polymer; (Poly)pentabromobenzyl acrylate; Poly(2,3,4,5,6-pentabromobenzyl acrylate); Polymer of 2,3,4,5,6-pentabromobenzyl acrylate; Pentabromobenzyl acrylate homopolymer; Ameribrom FR 1025; FR 1025; FR 1025P; PBB-PA</td></tr>
<tr><td colspan="2">Chemical Considerations: This alternative is a high molecular weight polymer. The high MW (MW >1,000) oligomers were assessed together using the Sustainable Futures (SF) polymer assessment criteria (U.S. EPA, 2010a).</td></tr>
<tr><td colspan="2">Polymeric: Yes
Oligomers: The formula for this polymer is $(C_{10}H_5Br_5O_2)_n$ and the average MW is approximately 80,000 daltons (NICNAS, 2001) with oligomers below 500 or 1,000 not expected.</td></tr>
<tr><td colspan="2">Metabolites, Degradates and Transformation Products: None</td></tr>
<tr><td>Analog: No analog
Endpoint(s) using analog values: Not applicable</td><td>Analog Structure: Not applicable</td></tr>
<tr><td colspan="2">Structural Alerts: None identified</td></tr>
<tr><td colspan="2">Risk Phrases: Not classified by Annex I Directive 67/548/EEC & IUCLID (Pakalin et al., 2007).</td></tr>
<tr><td colspan="2">Hazard and Risk Assessments: None identified</td></tr>
<tr><td colspan="2">U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory and is a commenced Premanufacture Notice substance. This chemical is exempt from reporting under the Chemical Data Reporting rule (CDR).</td></tr>
</table>

Brominated Polyacrylate CASRN 59447-57-3			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	180 (glass transition temperature) (Measured)	Sigma-Aldrich, 2011	The melting points reported cover a broad range and are anticipated to be formulation specific liquid-glass transition temperatures.
	190-220 (glass transition temperature) (Measured)	National Industrial Chemicals Notification and Assessment Scheme (NICNAS), 2001; Mack, 2004	
Boiling Point (°C)	>300 (Estimated)	Professional judgment	Cutoff value used for large, high MW solid.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010b	Cutoff value for large, high MW polymers according to SF polymer assessment guidance.
	<0.075 (Measured)	NICNAS, 2001	Reported in a secondary source. Insufficient information provided to assess the quality of the data.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	Professional judgment; EPA, 2010b	Cutoff value for large, high MW polymers according to SF polymer assessment guidance.
	3.5-3.8 (Measured)	NICNAS, 2001	Reported in a secondary source; value inconsistent with that expected for a highly halogenated polymer with a MW >10,000.
Log K_{ow}			No data located; polymers with a MW >1,000 are outside the domain of the available estimation methods.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.

Brominated Polyacrylate CASRN 59447-57-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Pyrolysis				No data located.
pH				No data located.
pK_a				No data located.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Brominated polyacrylate has a MW >1,000 and limited water solubility. There is no absorption expected for any route of exposure for this compound; therefore is not expected to be absorbed, distributed or metabolized in the body. The lack of absorption is expected to result in low hazard potential.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No absorption is expected for all routes of exposure (Estimated by analogy)	Professional judgment	Estimated based on professional judgment.
Acute Mammalian Toxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has a low potential for acute mammalian toxicity. No data located.**		
Acute Lethality	**Oral**	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
	Dermal			
	Inhalation			
Carcinogenicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have few to no residual monomers. Additionally, crosslinking, swellability, dispersability, reactive functional groups, inhalation potential, and hindered amine groups are not expected and therefore the carcinogenicity hazard for this chemical has a low potential for carcinogenicity. No data located.**		
	OncoLogic Results	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
	Carcinogenicity (Rat and Mouse)			
	Combined Chronic Toxicity/ Carcinogenicity			
Genotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has a low potential for genotoxicity. No data located.**		
	Gene Mutation *in vitro*	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
	Gene Mutation *in vivo*			
	Chromosomal Aberrations *in vitro*			

Brominated Polyacrylate CASRN 59447-57-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Chromosomal Aberrations *in vivo*			
	DNA Damage and Repair			
	Other (Mitotic Gene Conversion)			
Reproductive Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has a low potential for reproductive effects. No data located.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			
Developmental Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has a low potential for developmental effects. No data located.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			
	Postnatal Development			
Neurotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has a low potential for neurotoxicity. No data located.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.

Brominated Polyacrylate CASRN 59447-57-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects		**MODERATE: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability; however, because the number average molecular weight (MW_n) is >10,000 there is the possibility of lung overloading in dust forming conditions. No data located.**		
		Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
		This polymer MW_n is >10,000; potential for irreversible lung damage as a result of lung overloading (Estimated by analogy)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
Skin Sensitization		**LOW: Estimated to not have potential for skin sensitization based on expert judgment.**		
	Skin Sensitization	Low potential for skin sensitization. (Estimated)	Expert judgment	Estimated based on expert judgment.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Estimated to not have potential for eye irritation based on expert judgment.**		
	Eye Irritation	Low potential for skin sensitization. (Estimated)	Expert judgment	Estimated based on expert judgment.
Dermal Irritation		**LOW: Estimated to not have potential for dermal irritation based on expert judgment.**		
	Dermal Irritation	Low potential for skin sensitization. (Estimated)	Expert judgment	Estimated based on expert judgment.
Endocrine Activity		**This polymer is large, with a MW >1,000. It is not expected to have endocrine activity due to its limited bioavailability and inability to be readily metabolized in the body.**		
				No data located.
Immunotoxicity		**This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has a low potential for immunotoxicity. No data located.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010b	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		

Brominated Polyacrylate CASRN 59447-57-3			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Acute Toxicity	**LOW: Non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to display no effects at saturation (NES). These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard results in a low categorization for those materials that display NES.**		
Fish LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity	**LOW: Non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to display NES. These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard results in a low hazard categorization for those materials that display NES.**		
Fish ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.

Brominated Polyacrylate CASRN 59447-57-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that this polymer is anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of $<10^{-8}$ atm-m^3/mole indicates that it is not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that it is not anticipated to migrate from soil into groundwater and also has the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010b	High MW polymers are expected to have low vapor pressure and are not expected to undergo volatilization according to polymer assessment guidance.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; EPA, 2010b	High MW polymers are expected to adsorb strongly to soil and sediment according to SF polymer assessment guidance.
	Level III Fugacity Model			No data located.
Persistence		**VERY HIGH: This polymer is large, with a MW >1,000. It is expected to have negligible water solubility and limited bioavailability to microorganisms indicating that neither biodegradation nor hydrolysis are expected to be important removal processes in the environment. Although photodegradation of polybrominated benzenes has been observed, this process is not anticipated to lead to ultimate removal of the material. As a result, a half-life for this high MW polymer of >180 days leads to the potential for very high persistence.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment; EPA, 2010b	High MW polymers are expected to be non-biodegradable according to SF polymer assessment guidance.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
Soil	**Aerobic Biodegradation**			No data located.

Brominated Polyacrylate CASRN 59447-57-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Anaerobic Biodegradation			No data located.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.
Reactivity	**Photolysis**		Professional judgment	Bromine substituents are susceptible to photolysis; however this is expected to be a relatively slow process for brominated polyacrylate and is not anticipated to lead to ultimate removal of the material.
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.
Environmental Half-Life		>180 days (Estimated)	Professional judgment	The substance has a MW >1,000 and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. Other degradative processes under environmental conditions are also not anticipated.
Bioaccumulation		**LOW: Due to the large size and limited bioavailability of this polymer, it is of low potential for bioconcentration or bioaccumulation.**		
	Fish BCF	<100 (Estimated)	Professional judgment	Cutoff value for large, high MW, insoluble polymers according to SF polymer assessment guidance.

Brominated Polyacrylate CASRN 59447-57-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	BAF			No data located.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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Brominated Polystyrene

Screening Level Hazard Summary

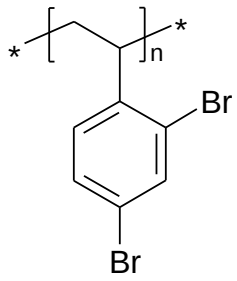
This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

[d] This hazard designation is driven by potential for lung overloading as a result of dust forming operations.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Brominated Polystyrene	88497-56-7	L	*L*	*L*	*L*	*L*	*L*	*M*[d]	*L*		L	*L*	*L*	*L*	*VH*	*L*

Brominated Polystyrene



Representative Structure

CASRN 88497-56-7

Molecular Weight (MW): 80,000 – 800,000 (Measured); 0%<1,000

Molecular Formula: $(C_8H_{8-m}Br_m)_n$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: This polymer with MW >1,000 and no low MW components is not amenable to SMILES notation.

Synonyms: Benzene, ethenyl-, homopolymer, brominated (TSCA Inventory); 2-Propenoic acid, (2,3,4,5,6-pentabromophenyl)methyl ester, homopolymer; Brominated ethenylbenzene homopolymer; Firemaster BP 41; Firemaster BP-411; Firemaster CP-44HF; FR 803; FR-803P; PDBS 80; Polystyrene, brominated; Pyro-Chek 68PB/BC; Saytex HP-775; Saytex HP-3010; Saytex HP-7010; Saytex HP-7010P; Saytex HP-7010G; Saytex HP-3010

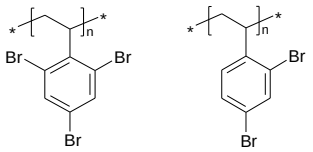
Chemical Considerations: This alternative is a high MW polymer. The number and locations of the bromines on the phenyl rings are unspecified and expected to be a variable mixture of mono, di, tri and tetra brominated materials. The ratio of m and n in the molecular formula $(C_8H_{8-m}Br_m)_n$ are product specific; although bromine content of 66-68% (m = 2.6-2.7) are typical (Mack 2004). These high MW oligomers were assessed together using the Sustainable Futures (SF) polymer assessment criteria (U.S. EPA 2010f). Closely related materials are indicated in the analog section

Polymeric: Yes
Oligomers: The general formula for this polymer is $(C_8H_{8-m}Br_m)_n$ and the average MW is 80,000 to 800,000 daltons (NICNAS, 2001) with oligomers MW <1,000 not expected.

Metabolites, Degradates and Transformation Products: None

Analog: Tribrominated polystyrene (CASRN 57137-10-7); Benzene, ethenyl-, ar-bromo derivs., homopolymers (CASRN 148993-99-1)
Endpoint(s) using analog values: Decomposition

Analog Structures:



Representative Structure
CASRN 57137-10-7 CASRN 148993-99-1

Structural Alerts: None identified
Risk Phrases: Not classified by Annex I Directive 67/548/EEC & IUCLID (Pakalin, Cole et al. 2007).
Hazard and Risk Assessments: None identified
U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory and is a commenced Premanufacture Notice substance. This chemical is exempt from reporting under the Chemical Data Reporting rule (CDR).

Brominated Polystyrene CASRN 88497-56-7			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	195 (glass transition temperature) (Measured)	Ioffe and Kampf, (2002)	The melting points reported cover a broad range and are anticipated to be formulation specific liquid-glass transition temperature.
	130-140 (glass transition temperature) (Measured)	Ioffe and Kampf, (2002)	
Boiling Point (°C)	Decomposes (Estimated by analogy)	Professional judgment	Based on data from 148993-99-1.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW polymers according to SF polymer assessment guidance.
Water Solubility (g/L)	$<10^{-6}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW non-ionic polymers according to SF polymer assessment guidance.
Log K_{ow}			No data located; polymers with a MW >1,000 are outside the domain of the available estimation methods.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.

Brominated Polystyrene CASRN 88497-56-7				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**There is no absorption expected for any route of exposure. This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No absorption is expected for any route of exposure (Estimated)	Professional judgment	Estimated based on professional judgment.
Acute Mammalian Toxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is of low potential for acute mammalian toxicity as confirmed by the available data.**		
Acute Lethality	**Oral**	Rat Oral LD_{50} >15,380 mg/kg	Industrial Bio-Test Laboratories, (1977b)	Guideline study.
	Dermal	Rabbit Dermal LD_{50} >3,038 mg/kg	Industrial Bio-Test Laboratories, (1977a)	Guideline study.
	Inhalation	Rat Inhalation (dust) 4-hour LC_{50} >5.25 mg/L No gross tissue changes were observed (a mean aerodynamic diameter of 3.8 ± 1.97 microns)	Springborn Labs Inc., (1991)	Guideline study.
Carcinogenicity		**LOW: This polymer is large, with a MW >1,000. Based on professional judgment, It is expected to have few to no residual monomers. Additionally, crosslinking, swellability, dispersability, reactive functional groups, inhalation potential, and hindered amine groups are not expected. Therefore there is low potential for carcinogenicity. No data located.**		
	OncoLogic Results **Carcinogenicity (Rat and Mouse)** **Combined Chronic Toxicity/ Carcinogenicity**	Limited bioavailability expected; crosslinking swellability, dispersability, reactive functional groups, inhalation potential, and hindered amine groups are not expected. (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.

Brominated Polystyrene CASRN 88497-56-7				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Genotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for genotoxicity. *In vitro* Ames test is negative for gene mutations.**		
	Gene Mutation *in vitro*	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
		Negative for gene mutations in *Salmonella typhimurium* strains TA1535, TA1537, TA1538, TA100, and TA98 with and without exogenous metabolic activation	Microbiological Associates, (1978)	Guideline study.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*			No data located.
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has a low potential for reproductive effects. No data located.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			

Brominated Polystyrene CASRN 88497-56-7				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has a low potential for developmental effects. No data located.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			
	Postnatal Development			
Neurotoxicity		**LOW: This polymer is large, with a MW > 1,000. It is expected to have limited bioavailability and therefore has a low potential for neurotoxicity. No data located.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
Repeated Dose Effects		**MODERATE: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability; however, because the number average molecular weight (MW_n) is >10,000 there is the possibility of lung overloading in dust forming conditions. No data located.**		
		Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
		This polymer MW_n is >10,000; potential for irreversible lung damage as a result of lung overloading (Estimated by analogy)	Professional judgment; EPA (2011j)0	Based on SF polymer assessment guidance.
Skin Sensitization		**LOW: Estimated to not have potential for skin sensitization based on expert judgment. No data located.**		
	Skin Sensitization	Not expected to be a skin sensitizer (Estimated)	Expert judgment	Estimated based on expert judgment.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Brominated polystyrene is a mild eye irritant in rabbits; irritation begins to clear within 24 hours and is completely cleared within 48 hours.**		

Brominated Polystyrene CASRN 88497-56-7				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Eye Irritation	Minimally irritating, rabbit clearing within 24 hours	Industrial Bio-Test Laboratories, (1977b)	Adequate, guideline study.
Dermal Irritation		**LOW: Estimated to not have potential for dermal irritation Available experimental data are inadequate to make a hazard designation for this endpoint.**		
	Dermal Irritation	Not expected to be a skin irritant (Estimated)	Expert judgment	Estimated based on expert judgment.
		Moderately irritating, rabbit. Skin reactions characterized by pale red to red, well-defined erythema and moderate to severe edema that subsided by 7 days. Slight desquamation at test skin site at 14 days. (Test substance was administered as a fine powder in a slurry containing 1.0% aqueous methylcellulose)	Industrial Bio-Test Laboratories, (1977a)	Result likely due to the presence of an impurity.
Endocrine Activity		**This polymer is large, with a MW >1,000. It is not expected to have endocrine activity due to its poor bioavailability and inability to readily metabolize in the body. No data located.**		
		Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
Immunotoxicity		**This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has a low potential for immunotoxicity. No data located.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**LOW: Non-ionic polymers with a MW > 1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers. These polymers display no effects at saturation (NES) because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Bioavailability is limited because this chemical cannot be absorbed through membranes due to large size.**		

Brominated Polystyrene CASRN 88497-56-7			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Fish LC_{50}	Fish (*Orizias latipes)* 48-hour TLm >500 mg/L	Nissan Ferro Organic Chem Inc, (1990)	Inadequate; OECD guidelines recommend study duration of 96-hours for this endpoint. Units are not applicable to screening methodology.
	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity	**LOW: Non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers. These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Bioavailability is limited because this chemical cannot be absorbed through membranes due to large size.**		
Fish ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Saltwater Invertebrate ChV			No data located.
Green Algae ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.

Brominated Polystyrene CASRN 88497-56-7				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that this polymer is anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of $<10^{-8}$ atm-m^3/mole indicates that it is not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that it is not anticipated to migrate from soil into groundwater and also has the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to have low vapor pressure and are not expected to undergo volatilization according to polymer assessment guidance.
	Sediment/Soil Adsorption/ Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; EPA, 2010	Cutoff value used for large, high MW polymers. High MW polymers are expected to adsorb strongly to soil and sediment according to SF polymer assessment guidance.
	Level III Fugacity Model			No data located.
Persistence		**VERY HIGH: This polymer is large, with a MW >1,000. It is expected to have negligible water solubility and poor bioavailability to microorganisms indicating that neither biodegradation nor hydrolysis are expected to be important removal processes in the environment. Although photodegradation of brominated polystyrenes has been observed, this process is not anticipated to lead to ultimate removal of the material. As a result, a half-life for this high MW polymer of >180 days leads to the potential for very high persistence.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to be non-biodegradable according to SF polymer assessment guidance.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation			No data located.

Brominated Polystyrene CASRN 88497-56-7				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.
Reactivity	**Photolysis**	Photodegradation observed based on a decreased MW of brominated polystyrene (Measured)	Kaeriyama, Shimura et al., (1972)	The bromine substituent is susceptible to photolysis; however, this is expected to be a relatively slow process for brominated polystyrene and is not anticipated to lead to ultimate removal of the material.
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.
Environmental Half-life		>180 days (Estimated)	Professional judgment	The substance has a MW >1,000 and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. Other degradative processes under environmental conditions are also not anticipated.
Bioaccumulation		**LOW: Due to the large size and water insolubility of this high MW polymer, it is of low potential for bioconcentration or bioaccumulation.**		
	Fish BCF	<100 (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW, insoluble polymers according to SF polymer assessment guidance.
	BAF			No data located.
	Metabolism in Fish			No data located.

Brominated Polystyrene CASRN 88497-56-7			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL MONITORING AND BIOMONITORING			
Environmental Monitoring	No data located.		
Ecological Biomonitoring	No data located.		
Human Biomonitoring	This chemical was not included in the NHANES biomonitoring report (CDC 2011)).		

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Springborn Labs Inc. (1991). Acute inhalation toxicity study in rats with Pyro-Chek LM (amended final report). EPA Document No. 86-910000862, Fiche No. OTS0530450.

Confidential Brominated Epoxy Polymer #1

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from estimation software and professional judgment.

[d] This hazard designation is driven by concern for lung overloading as a result of dust forming operations.

Chemical	CASRN	Human Health Effects										Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Confidential Brominated Epoxy Polymer #1	Confidential	*L*	*L*	*L*	*L*	*L*	*L*	*M* [d]	*L*		*L*	*L*	*L*	*L*	*VH*	*L*

Confidential Brominated Epoxy Polymer #1

	CASRN: Confidential CASRN
	MW: Average MW 50,000; 0% MW <1,000
	MF: Confidential MF
	Physical Forms: **Neat:** Solid
	Use: Flame retardant
SMILES: This mixture containing confidential material is not amenable to the generation of a single SMILES notation.	
Synonyms: Polyquel 240	
Chemical Considerations: This alternative is a high MW polymer. These high molecular weight oligomers, with a MW > 1,000, are assessed using the Sustainable Futures (SF) polymer assessment criteria in this report (U.S. EPA, 2010).	
Polymeric: Yes **Oligomers:** The confidential commercial product is comprised of high molecular weight epoxy-terminated oligomers.	
Metabolites, Degradates and Transformation Products: None	
Analog: Confidential **Endpoint(s) using analog values:** Boiling point	**Structure:** Not applicable
Structural Alerts: None identified	
Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).	
Hazard and Risk Assessments: None identified	
U.S. EPA TSCA Regulatory Status: The components of this mixture are listed on the Toxic Substances Control Act (TSCA) Inventory and are exempt from reporting under the Chemical Data Reporting rule (CDR).	

Confidential Brominated Epoxy Polymer #1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	145-155 (Measured)	Warmington, 2010	Formulation specific liquid-glass transition temperatures for the commercial product Polyquel 240.
Boiling Point (°C)	Decomposes (Estimated)	Professional judgment	Based on analogy to a confidential polymer with a similar structure and functional groups.
	>300 (Estimated)	Professional judgment	Cutoff value used for large, high molecular weight solids.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high molecular weight non-ionic polymers according to SF polymer assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$(Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high molecular weight non-ionic polymers according to SF polymer assessment guidance.
Log K_{ow}			No data; polymers with a MW >1,000 are outside the domain of the available estimation methods.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.

Confidential Brominated Epoxy Polymer #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**There is no absorption expected for any route of exposure. This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral**	No absorption is expected for any route of exposure (Estimated)	Professional judgment	Estimated based on professional judgment.
Acute Mammalian Toxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is of low potential for acute mammalian toxicity.**		
Acute Lethality	**Oral**	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Dermal			
	Inhalation			
Carcinogenicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have few to no residual monomers, crosslinking, swellability, dispersability, potential for inhalation, nor hindered amine groups and therefore has low potential for carcinogenicity.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Chronic Toxicity/ Carcinogenicity			
Genotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for genotoxicity.**		
	Gene Mutation *in vitro*	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Gene Mutation *in vivo*			
	Chromosomal Aberrations *in vitro*			
	Chromosomal Aberrations *in vivo*			
	DNA Damage and Repair			

Confidential Brominated Epoxy Polymer #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Other (Mitotic Gene Conversion)			
Reproductive Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for reproductive effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			
Developmental Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for developmental effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			
	Postnatal Development			
Neurotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for neurotoxicity.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.

Confidential Brominated Epoxy Polymer #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects		**MODERATE: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability; however, because the MW_n is >10,000 there is the possibility of lung overloading in dust forming conditions.**		
		This polymer MW_n is >10,000; potential for irreversible lung damage as a result of lung overloading (Estimated)	Professional judgment; EPA, 2011	Based on SF polymer assessment guidance.
Skin Sensitization		**LOW: Estimated not to have potential for skin sensitization based on expert judgment. No data located.**		
	Skin Sensitization	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Estimated not to have potential for eye irritation based on expert judgment. No data located.**		
	Eye Irritation	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Dermal Irritation		**LOW: Estimated not to have potential for dermal irritation based on expert judgment. No data located.**		
	Dermal Irritation	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Endocrine Activity		**This polymer is large, with a MW >1,000. It is not expected to have endocrine activity due to its poor bioavailability and inability to be readily metabolized in the body.**		
		Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
Immunotoxicity		**This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for immunotoxicity.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**LOW: Non-ionic polymers with a MW >1,000 and negligible water solubility are estimated to display no effects at saturation (NES). These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for those materials that display NES.**		

Confidential Brominated Epoxy Polymer #1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Fish LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity	**LOW: Non-ionic polymers with a MW >1,000 and negligible water solubility are estimated to display NES. These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for those materials that display NES.**		
Fish ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.

Confidential Brominated Epoxy Polymer #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that this polymer is anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of <10^{-8} atm-m^3/mole indicates that it is not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that it is not anticipated to migrate from soil into groundwater and also has the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	<10^{-8} (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to have low vapor pressure and are not expected to undergo volatilization according to polymer assessment guidance.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; EPA, 2010	Cutoff value used for large, high MW polymers. High MW polymers are expected to adsorb strongly to soil and sediment according to SF polymer assessment guidance.
	Level III Fugacity Model			No data located.
Persistence		**VERY HIGH: This polymer is large, with a MW >1,000. It is expected to have negligible water solubility and poor bioavailability to microorganisms indicating that neither biodegradation nor hydrolysis are expected to be important removal processes in the environment. Although debromination by photodegradation of polybrominated benzenes has been observed, this process is not anticipated to lead to ultimate removal of the material. As a result, a half-life for this high MW polymer of >180 days leads to a potential for very high persistence.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to be non-biodegradable according to SF polymer assessment guidance.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.

Confidential Brominated Epoxy Polymer #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation			No data located.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Professional judgment	Bromine substituents may be susceptible to photolysis in the environment; however, this is expected to be a relatively slow process for a high MW brominated epoxy polymer and is not anticipated to result in the ultimate degradation of this substance.
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.
Environmental Half-Life		>180 days (Estimated)	Professional judgment	The substance is a high MW polymer and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to undergo removal by other degradative processes under environmental conditions.

Confidential Brominated Epoxy Polymer #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Bioaccumulation		**LOW: Due to the large size and limited bioavailability of the high MW confidential brominated epoxy polymer #1, it is of low potential for bioconcentration or bioaccumulation.**		
	Fish BCF	<100 (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW, insoluble polymers according to SF polymer assessment guidance.
	BAF			No data located.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

CDC (Centers for Disease Control and Prevention). *Fourth national report on human exposure to environmental chemicals, updated tables*. Department of Health and Human Services. **2011.** http://www.cdc.gov/exposurereport/pdf/Updated_Tables.pdf (accessed on May 10, 2011).

ESIS (European chemical Substances Information System) Classification, labeling and packaging of dangerous substances annex VI to regulation (EC) No 1272/2008 [Online]. http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=cla (accessed on May 10, 2011).

Sustainable Futures Summary Assessment. *Interpretive Assistance Document for Assessment of Polymers.* U.S. Environmental Protection Agency: Washington D.C. 2010. http://www.epa.gov/oppt/sf/pubs/iad_polymers_042010.pdf as of September 2, 2011.

Warmington, A (ed). Speciality Chemicals Magazine. Quartz business Media ltd., September 2010, v.30(9) p. 40-1. **2010**.

Confidential Brominated Epoxy Polymer #2

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame-retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from estimation software and professional judgment.

[d] This hazard designation is driven by concern for lung overloading as a result of dust forming operations.

♦ Different formulations of the commercial product are available. One of these many formulations has an average MW of ~1,600 and contains significant amounts of lower MW components. These lower MW components are primarily unchanged starting materials that have hazard potentials different than the polymeric flame retardant, as follows: VERY HIGH- Estimated potential for bioaccumulation; HIGH-Experimental concern for acute aquatic toxicity; HIGH-Estimated potential for chronic aquatic toxicity; MODERATE-Experimental concern for developmental; and MODERATE-Estimated potential for carcinogencity, genotoxicity, repeated dose, reproductive, and skin and respiratory sensitization toxicity.

		Human Health Effects											Aquatic Toxicity		Environmental Fate	
Chemical	CASRN	Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Confidential Brominated Epoxy Polymer #2	Confidential	*L*	*L*♦	*L*♦	*L*♦	*L*♦	*L*	*M*♦ [d]	*L*♦	♦	*L*	*L*	*L*♦	*L*♦	*VH*	*L*♦

Confidential Brominated Epoxy Polymer #2

	CASRN: Confidential CASRNs
	MW: Average MW 40,300; <5% MW <1,000
	MF: Confidential MFs
	Physical Forms: **Neat:** Solid
	Use: Flame retardant
SMILES: This confidential material is not amenable to the generation of a single SMILES notation.	
Synonyms: Polyquel 241	
Chemical Considerations: This alternative is a polymer; the majority of this polymer is comprised of high molecular weight oligomers. The higher molecular weight oligomers, with a MW > 1,000, are assessed together using the Sustainable Futures (SF) polymer assessment criteria in this report (U.S. EPA, 2010). However, it should be noted that <5% of this commercial product consists of components with a MW <1,000. A summary of the hazards of the MW <1,000 materials are provided in Table 4-4 as a footnote (♦).	
Polymeric: Yes **Oligomers:** The majority of this confidential commercial product (>95%) is comprised of high molecular weight epoxy-terminated oligomers.	
Metabolites, Degradates and Transformation Products: None	
Analog: Confidential **Endpoint(s) using analog values:** Boiling point	**Analog Structure:** Not applicable
Structural Alerts: None identified	
Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).	
Exposure Considerations: Not expected to be distinguishing.	
Life-Cycle Considerations: Not expected to be distinguishing.	
Hazard and Risk Assessments: None identified	
U.S. EPA TSCA Regulatory Status: The components of this mixture are listed on the Toxic Substances Control Act (TSCA) Inventory and are exempt from reporting under the Chemical Data Reporting rule (CDR).	

Confidential Brominated Epoxy Polymer #2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	145-155 (Measured)	Warmington, 2010	Formulation specific liquid-glass transition temperatures for the commercial product Polyquel 241.
Boiling Point (°C)	Decomposes	ICL Industrial, 2011	Based on analogy to a confidential polymer with a similar structure and functional groups.
	>300 (Estimated)	Professional judgment	Cutoff value used for large, high molecular weight solids.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high molecular weight non-ionic polymers according to SF polymer assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high molecular weight non-ionic polymers according to SF polymer assessment guidance.
Log K_{ow}			No data; polymers with a MW >1,000 are outside the domain of the available estimation methods.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.

Confidential Brominated Epoxy Polymer #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**There is no absorption expected for any route of exposure. This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body. However, there are formulations of the commercial product available that may contains significant amounts of lower MW components; absorption may occur more readily in this case.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral**	No absorption is expected for any route of exposure (Estimated)	Professional judgment	Estimated based on professional judgment.
Acute Mammalian Toxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is of low potential for acute mammalian toxicity.**		
Acute Lethality	**Oral**	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Dermal			
	Inhalation			
Carcinogenicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have few to no residual monomers, crosslinking, swellability, dispersability, potential for inhalation, nor hindered amine groups and therefore has low potential for carcinogenicity.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Chronic Toxicity/ Carcinogenicity			
Genotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for genotoxicity.**		
	Gene Mutation *in vitro*	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Gene Mutation *in vivo*			
	Chromosomal Aberrations *in vitro*			
	Chromosomal Aberrations *in vivo*			

Confidential Brominated Epoxy Polymer #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	DNA Damage and Repair			
	Other (Mitotic Gene Conversion)			
Reproductive Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for reproductive effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			
Developmental Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for developmental effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			
	Postnatal Development			
Neurotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for neurotoxicity.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.

Confidential Brominated Epoxy Polymer #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects		**MODERATE: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability; however, because the MW_n is >10,000 there is the possibility of lung overloading in dust forming conditions.**		
		This polymer MW_n is >10,000; potential for irreversible lung damage as a result of lung overloading (Estimated)	Professional judgment; EPA, 2011	Based on SF polymer assessment guidance.
Skin Sensitization		**LOW: Estimated not to have potential for skin sensitization based on expert judgment. No data located.**		
	Skin Sensitization	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Estimated not to have potential for eye irritation based on expert judgment. No data located.**		
	Eye Irritation	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Dermal Irritation		**LOW: Estimated not to have potential for dermal irritation based on expert judgment. No data located.**		
	Dermal Irritation	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Endocrine Activity		**This polymer is large, with a MW >1,000. It is not expected to have endocrine activity due to its poor bioavailability and inability to be readily metabolized in the body.**		
		Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
Immunotoxicity		**This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for immunotoxicity.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**LOW: Non-ionic polymers with a MW >1,000 and negligible water solubility are estimated to display no effects at saturation (NES). These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for those materials that display NES.**		

Confidential Brominated Epoxy Polymer #2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Fish LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity	**LOW: Non-ionic polymers with a MW >1,000 and negligible water solubility are estimated to display NES. These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for those materials that display NES.**		
Fish ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.

Confidential Brominated Epoxy Polymer #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that this polymer is anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of <10^{-8} atm-m^3/mole indicates that it is not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that it is not anticipated to migrate from soil into groundwater and also has the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	<10^{-8} (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to have low vapor pressure and are not expected to undergo volatilization according to polymer assessment guidance.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; EPA, 2010	Cutoff value used for large, high MW polymers. High MW polymers are expected to adsorb strongly to soil and sediment according to SF polymer assessment guidance.
	Level III Fugacity Model			No data located.
Persistence		**VERY HIGH: This polymer is large, with a MW >1,000. It is expected to have negligible water solubility and poor bioavailability to microorganisms indicating that neither biodegradation nor hydrolysis are expected to be important removal processes in the environment. Although debromination by photodegradation of polybrominated benzenes has been observed, this process is not anticipated to lead to ultimate removal of the material. As a result, a half-life for this high MW polymer of >180 days leads to a potential for very high persistence.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to be non-biodegradable according to SF polymer assessment guidance.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.

Confidential Brominated Epoxy Polymer #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation			No data located.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Professional judgment	Bromine substituents may be susceptible to photolysis in the environment; however, this is expected to be a relatively slow process for a high MW brominated epoxy polymer and is not anticipated to result in the ultimate degradation of this substance.
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.
Environmental Half-Life		>180 days (Estimated)	Professional judgment	The substance is a high MW polymer and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to undergo removal by other degradative processes under environmental conditions.

Confidential Brominated Epoxy Polymer #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Bioaccumulation		**LOW: Due to the large size and limited bioavailability of the confidential brominated epoxy polymer #2, it is of low potential for bioconcentration or bioaccumulation.**		
	Fish BCF	<100 (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW, insoluble polymers according to SF polymer assessment guidance.
	BAF			No data located.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

CDC (Centers for Disease Control and Prevention). *Fourth national report on human exposure to environmental chemicals, updated tables*. Department of Health and Human Services. **2011.** http://www.cdc.gov/exposurereport/pdf/Updated_Tables.pdf (accessed on May 10, 2011).

[Polymer Assessment Guidance] EPA (Environmental Protection Agency). Sustainable Futures Summary Assessment. *Interpretive Assistance Document for Assessment of Polymers*. U.S. Environmental Protection Agency: Washington D.C. **2010**. http://www.epa.gov/oppt/sf/pubs/iad_polymers_042010.pdf as of September 2, 2011.

ESIS (European chemical Substances Information System) Classification, labeling and packaging of dangerous substances annex VI to regulation (EC) No 1272/2008 [Online]. http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=cla (accessed on May 10, 2011).

Sustainable Futures Summary Assessment. *Interpretive Assistance Document for Assessment of Polymers*. U.S. Environmental Protection Agency: Washington D.C. 2010. http://www.epa.gov/oppt/sf/pubs/iad_polymers_042010.pdf as of September 2, 2011.

Warmington, A (ed). Speciality Chemicals Magazine. Quartz business Media ltd., September 2010, v.30(9) p. 40-1. **2010**.

Confidential Brominated Epoxy Polymer Mixture #1

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from estimation software and professional judgment.

[d] This hazard designation is driven by concern for lung overloading as a result of dust forming operations.

♦ Different formulations of the commercial product are available. One of these many formulations has an average MW of ~1,600 and contains significant amounts of lower MW components. These lower MW components are primarily unchanged starting materials that have hazard potentials different than the polymeric flame retardant, as follows: VERY HIGH- Estimated potential for bioaccumulation; HIGH-Experimental concern for acute aquatic toxicity; HIGH-Estimated potential for chronic aquatic toxicity; MODERATE-Experimental concern for developmental; and MODERATE-Estimated potential for carcinogencity, genotoxicity, repeated dose, reproductive, and skin and respiratory sensitization toxicity.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Confidential Brominated Epoxy Polymer Mixture #1	Confidential	*L*	*L*♦	*L*♦	*L*♦	*L*♦	*L*	*M*♦ [d]	*L*♦	*L*	*L*	♦	*L*♦	*L*♦	*VH*	*L*♦

Confidential Brominated Epoxy Polymer Mixture #1

<table>
<tr><td colspan="2" rowspan="4"></td><td>CASRN: Confidential CASRNs</td></tr>
<tr><td>MW: Average MW 61,200;
<1% MW <1,000</td></tr>
<tr><td>MF: Confidential MFs</td></tr>
<tr><td>Physical Forms:
Neat: Solid</td></tr>
<tr><td colspan="2">Use: Flame retardant</td></tr>
<tr><td colspan="3">SMILES: This mixture containing confidential material is not amenable to the generation of a single SMILES notation.</td></tr>
<tr><td colspan="3">Synonyms: Polyquel 145</td></tr>
<tr><td colspan="3">Chemical Considerations: This alternative is a confidential mixture comprised of three high molecular weight polymers. All components are high molecular weight oligomers, with a MW > 1,000, and are assessed using the Sustainable Futures (SF) polymer assessment criteria (U.S. EPA, 2010). The final hazard evaluation, presented in Table 4-4, is based on the most hazardous material typically present in the commercial product, using a conservative approach. However, it should be noted that <1% of this commercial product consists of components with a MW <1,000. A summary of the hazards of the MW <1,000 materials are provided in Table 4-4 as a footnote (♦).</td></tr>
<tr><td colspan="3">Polymeric: Yes
Oligomers: This commercial product is a confidential mixture comprised of three high molecular weight polymers: a brominated epoxy polymer, an end capped brominated epoxy polymer and a brominated polyacrylate.</td></tr>
<tr><td colspan="3">Metabolites, Degradates and Transformation Products: None</td></tr>
<tr><td colspan="2">Analog: Confidential
Endpoint(s) using analog values: Boiling point</td><td>Analog Structure: Confidential structure</td></tr>
<tr><td colspan="3">Structural Alerts: None identified</td></tr>
<tr><td colspan="3">Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).</td></tr>
<tr><td colspan="3">Hazard and Risk Assessments: None identified</td></tr>
<tr><td colspan="3">U.S. EPA TSCA Regulatory Status: The components of this mixture are listed on the Toxic Substances Control Act (TSCA) Inventory and were either existing chemicals or commenced after PMN review. Some components are exempt from reporting under the Chemical Data Reporting rule (CDR).</td></tr>
</table>

Confidential Brominated Epoxy Polymer Mixture #1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)			No data located.
Boiling Point (°C)	Decomposes (Estimated)	Professional judgment	Based on analogy to a confidential polymer with a similar structure and functional groups.
	>300 (Estimated)	Professional judgment	Cutoff value used for large, high molecular weight solids.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high molecular weight non-ionic polymers according to SF polymer assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high molecular weight non-ionic polymers according to SF polymer assessment guidance.
Log K_{ow}			No data located. Polymers with a MW >1,000 are outside the domain of the available estimation methods.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Dissociation is not expected; the chemical does not contain ionizable functional groups (Estimated)	Professional judgment	This polymer mixture does not contain functional groups that would be expected to ionize.
pK_a	Dissociation is not expected; the chemical does not contain ionizable functional groups (Estimated)	Professional judgment	This polymer mixture does not contain functional groups that would be expected to ionize.

Confidential Brominated Epoxy Polymer Mixture #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**There is no absorption expected for any route of exposure. These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral**	No absorption is expected for any route of exposure (Estimated)	Professional judgment	Estimated based on professional judgment.
Acute Mammalian Toxicity		**LOW: These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore are of low potential for acute mammalian toxicity.**		
Acute Lethality	**Oral**	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Dermal			
	Inhalation			
Carcinogenicity		**LOW: These polymers are large, with MW >1,000. They are expected to have few to no residual monomers, crosslinking, swellability, dispersability, potential for inhalation, nor hindered amine groups and therefore have low potential for carcinogenicity.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Chronic Toxicity/ Carcinogenicity			
Genotoxicity		**LOW: These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore have low potential for genotoxicity.**		
	Gene Mutation *in vitro*	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Gene Mutation *in vivo*			
	Chromosomal Aberrations *in vitro*			
	Chromosomal Aberrations *in vivo*			
	DNA Damage and Repair			

Confidential Brominated Epoxy Polymer Mixture #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Other (Mitotic Gene Conversion)			
Reproductive Effects		**LOW: These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore have low potential for reproductive effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			
Developmental Effects		**LOW: These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore have low potential for developmental effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			
	Postnatal Development			
Neurotoxicity		**LOW: These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore have low potential for neurotoxicity.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.

Confidential Brominated Epoxy Polymer Mixture #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects		**MODERATE: These polymers are large, with MW >1,000. They are expected to have limited bioavailability; however, because the MW_n is >10,000 there is the possibility of lung overloading in dust forming conditions.**		
		The polymer mixture MW_n is >10,000; potential for irreversible lung damage as a result of lung overloading (Estimated)	Professional judgment; EPA, 2011	Based on SF polymer assessment guidance.
Skin Sensitization		**LOW: Estimated not to have potential for skin sensitization based on expert judgment. No data located.**		
	Skin Sensitization	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Estimated not to have potential for eye irritation based on expert judgment. No data located.**		
	Eye Irritation	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Dermal Irritation		**LOW: Estimated not to have potential for dermal irritation based on expert judgment. No data located.**		
	Dermal Irritation	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Endocrine Activity		**These polymers are large, with MW >1,000. They are not expected to have endocrine activity due to poor bioavailability and inability to be readily metabolized in the body.**		
		Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
Immunotoxicity		**These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore have low potential for immunotoxicity.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**LOW: Non-ionic polymers with a MW >1,000 and negligible water solubility are estimated to display no effects at saturation (NES). These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for those materials that display NES.**		

Confidential Brominated Epoxy Polymer Mixture #1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Fish LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity	**LOW: Non-ionic polymers with a MW >1,000 and negligible water solubility are estimated to display NES. These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for those materials that display NES.**		
Fish ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.

Confidential Brominated Epoxy Polymer Mixture #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that these polymers are anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of $<10^{-8}$ atm-m^3/mole indicates that they are not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that they are not anticipated to migrate from soil into groundwater and also have the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to have low vapor pressure and are not expected to undergo volatilization according to polymer assessment guidance.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; EPA, 2010	Cutoff value used for large, high MW polymers. High MW polymers are expected to adsorb strongly to soil and sediment according to SF polymer assessment guidance.
	Level III Fugacity Model			No data located.
Persistence		**VERY HIGH: These polymers are large, with MW >1,000. They are expected to have negligible water solubility and poor bioavailability to microorganisms indicating that neither biodegradation nor hydrolysis are expected to be important removal processes in the environment. Although debromination by photodegradation of polybrominated benzenes has been observed, this process is not anticipated to lead to ultimate removal of the material. As a result, a half-life for these high MW polymer of >180 days leads to a potential for very high persistence.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to be non-biodegradable according to SF polymer assessment guidance.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.

Confidential Brominated Epoxy Polymer Mixture #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation			No data located.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Professional judgment	Bromine substituents may be susceptible to photolysis in the environment; however, this is expected to be a relatively slow process for a high MW brominated epoxy polymer and is not anticipated to result in the ultimate degradation of this substance.
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.
Environmental Half-Life		>180 days (Estimated)	Professional judgment	The substance is a high MW polymer and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to undergo removal by other degradative processes under environmental conditions.

Confidential Brominated Epoxy Polymer Mixture #1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Bioaccumulation		**LOW: Due to the large size and limited bioavailability of the high MW confidential brominated epoxy polymer mixture #1, it is of low potential for bioconcentration or bioaccumulation.**		
	Fish BCF	<100 (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW, insoluble polymers according to SF polymer assessment guidance.
	BAF			No data located.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

CDC (Centers for Disease Control and Prevention). *Fourth national report on human exposure to environmental chemicals, updated tables*. Department of Health and Human Services. **2011.** http://www.cdc.gov/exposurereport/pdf/Updated_Tables.pdf (accessed on May 10, 2011).

[Polymer Assessment Guidance] EPA (Environmental Protection Agency). Sustainable Futures Summary Assessment. *Interpretive Assistance Document for Assessment of Polymers.* U.S. Environmental Protection Agency: Washington D.C. **2010**. http://www.epa.gov/oppt/sf/pubs/iad_polymers_042010.pdf as of September 2, 2011

ESIS (European chemical Substances Information System) Classification, labeling and packaging of dangerous substances annex VI to regulation (EC) No 1272/2008 [Online]. http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=cla (accessed on May 10, 2011).

Confidential Brominated Epoxy Polymer Mixture #2

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame-retardant (FR) chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts.

The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from estimation software and professional judgment.

[d] This hazard designation is driven by concern for lung overloading as a result of dust forming operations.

♦ Different formulations of the commercial product are available. One of these many formulations has an average MW of ~1,600 and contains significant amounts of lower MW components. These lower MW components are primarily unchanged starting materials that have hazard potentials different than the polymeric flame retardant, as follows: VERY HIGH- Estimated potential for bioaccumulation; HIGH-Experimental concern for acute aquatic toxicity; HIGH-Estimated potential for chronic aquatic toxicity; MODERATE-Experimental concern for developmental; and MODERATE-Estimated potential for carcinogencity, genotoxicity, repeated dose, reproductive, and skin and respiratory sensitization toxicity.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Confidential Brominated Epoxy Polymer Mixture #2	Confidential	*L*	*L*♦	*L*♦	*L*♦	*L*♦	*L*	*M*♦ [d]	*L*♦	♦	*L*	*L*	*L*♦	*L*♦	*VH*	*L*♦

Confidential Brominated Epoxy Polymer Mixture #2

<table>
<tr><td colspan="2" rowspan="4"></td><td>CASRN: Confidential CASRNs</td></tr>
<tr><td>MW: Average MW 45,000;
<2% MW <1,000</td></tr>
<tr><td>MF: Confidential MFs</td></tr>
<tr><td>Physical Forms:
Neat: Solid</td></tr>
<tr><td colspan="2">Use: Flame retardant</td></tr>
<tr><td colspan="3">SMILES: This mixture containing confidential material is not amenable to the generation of a single SMILES notation.</td></tr>
<tr><td colspan="3">Synonyms: Polyquel 146</td></tr>
<tr><td colspan="3">Chemical Considerations: This alternative is a confidential mixture comprised of two high molecular weight polymers: a brominated epoxy polymer and a brominated polyacrylate. Both components are high molecular weight oligomers, with a MW > 1,000, and are assessed using the Sustainable Futures (SF) polymer assessment criteria (U.S. EPA, 2010). The final hazard evaluation, presented in Table 4-4 is based on the most hazardous material typically present in the commercial product, using a conservative approach. However, it should be noted that <2% of this commercial product consists of components with a MW <1,000. A summary of the hazards of the MW <1,000 materials are provided in Table 4-4 as a footnote (♦).</td></tr>
<tr><td colspan="3">Polymeric: Yes
Oligomers: This commercial product is a confidential mixture comprised of two high molecular weight polymers: a brominated epoxy polymer and a brominated polyacrylate.</td></tr>
<tr><td colspan="3">Metabolites, Degradates and Transformation Products: None</td></tr>
<tr><td colspan="2">Analog: Confidential
Endpoint(s) using analog values: Boiling point</td><td>Analog Structure: Confidential structure</td></tr>
<tr><td colspan="3">Structural Alerts: None identified</td></tr>
<tr><td colspan="3">Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).</td></tr>
<tr><td colspan="3">Hazard and Risk Assessments: None identified</td></tr>
<tr><td colspan="3">U.S. EPA TSCA Regulatory Status: The components of this mixture are listed on the Toxic Substances Control Act (TSCA) Inventory and were either existing chemicals on commenced after PMN review.</td></tr>
</table>

Confidential Brominated Epoxy Polymer Mixture #2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)			No data
Boiling Point (°C)	Decomposes (Estimated)	Professional judgment	Based on analogy to a confidential polymer with a similar structure and functional groups.
	>300 (Estimated)	Professional judgment	Cutoff value used for large, high molecular weight.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment, EPA, 2010	Cutoff value for large, high molecular weight non-ionic polymers according to SF polymer assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high molecular weight non-ionic polymers according to SF polymer assessment guidance.
Log K_{ow}			No data; polymers with a MW >1,000 are outside the domain of the available estimation methods.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Dissociation is not expected; the chemical does not contain ionizable functional groups (Estimated)	Professional judgment	This polymer mixture does not contain functional groups that would be expected to ionize.
pK_a	Dissociation is not expected; the chemical does not contain ionizable functional groups (Estimated)	Professional judgment	This polymer mixture does not contain functional groups that would be expected to ionize.

Confidential Brominated Epoxy Polymer Mixture #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**There is no absorption expected for any route of exposure. These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral**	No absorption is expected for any route of exposure (Estimated)	Professional judgment	Estimated based on professional judgment.
Acute Mammalian Toxicity		**LOW: These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore are of low potential for acute mammalian toxicity.**		
Acute Lethality	**Oral**	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Dermal			
	Inhalation			
Carcinogenicity		**LOW: These polymers are large, with MW >1,000. They are expected to have few to no residual monomers, crosslinking, swellability, dispersability, potential for inhalation, nor hindered amine groups and therefore have low potential for carcinogenicity.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Chronic Toxicity/ Carcinogenicity			

Confidential Brominated Epoxy Polymer Mixture #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Genotoxicity		**LOW: These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore have low potential for genotoxicity.**		
	Gene Mutation *in vitro*	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Gene Mutation *in vivo*			
	Chromosomal Aberrations *in vitro*			
	Chromosomal Aberrations *in vivo*			
	DNA Damage and Repair			
	Other (Mitotic Gene Conversion)			
Reproductive Effects		**LOW: These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore have low potential for reproductive effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			

Confidential Brominated Epoxy Polymer Mixture #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**LOW: These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore have low potential for developmental effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			
	Postnatal Development			
Neurotoxicity		**LOW: These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore have low potential for neurotoxicity.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
Repeated Dose Effects		**MODERATE: These polymers are large, with MW >1,000. They are expected to have limited bioavailability; however, because the MW_n is >10,000 there is the possibility of lung overloading in dust forming conditions.**		
		The polymer mixture MW_n is >10,000; potential for irreversible lung damage as a result of lung overloading (Estimated)	Professional judgment; EPA, 2011	Based on SF polymer assessment guidance.
Skin Sensitization		**LOW: Estimated not to have potential for skin sensitization based on expert judgment. No data located.**		
	Skin Sensitization	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Estimated not to have potential for eye irritation based on expert judgment. No data located.**		
	Eye Irritation	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Dermal Irritation		**LOW: Estimated not to have potential for dermal irritation based on expert judgment. No data located.**		
	Dermal Irritation	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.

Confidential Brominated Epoxy Polymer Mixture #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Endocrine Activity		**These polymers are large, with MW >1,000. They are not expected to have endocrine activity due to poor bioavailability and inability to be readily metabolized in the body.**		
		Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
Immunotoxicity		**These polymers are large, with MW >1,000. They are expected to have limited bioavailability and therefore have low potential for immunotoxicity.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**LOW: Non-ionic polymers with a MW >1,000 and negligible water solubility are estimated to display no effects at saturation (NES). These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for those materials that display NES.**		
Fish LC_{50}		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid LC_{50}		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity		**LOW: Non-ionic polymers with a MW >1,000 and negligible water solubility are estimated to display NES. These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for those materials that display NES.**		

Confidential Brominated Epoxy Polymer Mixture #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Fish ChV		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid ChV		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae ChV		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that these polymers are anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of $<10^{-8}$ atm-m^3/mole indicates that they are not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that they are not anticipated to migrate from soil into groundwater and also have the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to have low vapor pressure and are not expected to undergo volatilization according to polymer assessment guidance.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; EPA, 2010	Cutoff value used for large, high MW polymers. High MW polymers are expected to adsorb strongly to soil and sediment according to SF polymer assessment guidance.
	Level III Fugacity Model			No data located.

Confidential Brominated Epoxy Polymer Mixture #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Persistence		**VERY HIGH: These polymers are large, with MW >1,000. They are expected to have negligible water solubility and poor bioavailability to microorganisms indicating that neither biodegradation nor hydrolysis are expected to be important removal processes in the environment. Although debromination by photodegradation of polybrominated benzenes has been observed, this process is not anticipated to lead to ultimate removal of the material. As a result, a half-life for these high MW polymer of >180 days leads to a potential for very high persistence.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to be non-biodegradable according to SF polymer assessment guidance.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation			No data located.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Professional judgment	Bromine substituents may be susceptible to photolysis in the environment; however, this is expected to be a relatively slow process for a high MW brominated epoxy polymer and is not anticipated to result in the ultimate degradation of this substance.

Confidential Brominated Epoxy Polymer Mixture #2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.
Environmental Half-Life		>180 days (Estimated)	Professional judgment	The substance is a high MW polymer and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to undergo removal by other degradative processes under environmental conditions.
Bioaccumulation		**LOW: Due to the large size and limited bioavailability of the high MW confidential brominated epoxy polymer mixture #2, it is of low potential for bioconcentration or bioaccumulation.**		
	Fish BCF	<100 (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW, insoluble polymers according to SF polymer assessment guidance.
	BAF			No data located.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

CDC (Centers for Disease Control and Prevention). *Fourth national report on human exposure to environmental chemicals, updated tables*. Department of Health and Human Services. **2011.** http://www.cdc.gov/exposurereport/pdf/Updated_Tables.pdf (accessed on May 10, 2011).

[Polymer Assessment Guidance] EPA (Environmental Protection Agency). Sustainable Futures Summary Assessment. *Interpretive Assistance Document for Assessment of Polymers*. U.S. Environmental Protection Agency: Washington D.C. **2010**. http://www.epa.gov/oppt/sf/pubs/iad_polymers_042010.pdf as of September 2, 2011.

ESIS (European chemical Substances Information System) Classification, labeling and packaging of dangerous substances annex VI to regulation (EC) No 1272/2008 [Online]. http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=cla (accessed on May 10, 2011).

Confidential Brominated Polymer

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

¤ This alternative may contain impurities. These impurities have hazard designations that differ from the flame retardant alternative, Confidential Brominated Polymer, as follows, based on experimental data: HIGH for human health, HIGH for aquatic toxicity, VERY HIGH for bioaccumulation, and VERY HIGH for persistence.

T This chemical is subject to testing in an EPA consent order.

		Human Health Effects											Aquatic Toxicity		Environmental Fate	
Chemical	**CASRN**	**Acute Toxicity**	**Carcinogenicity**	**Genotoxicity**	**Reproductive**	**Developmental**	**Neurological**	**Repeated Dose**	**Skin Sensitizer**	**Respiratory Sensitization**	**Eye Irritation**	**Dermal Irritation**	**Acute**	**Chronic**	**Persistence**	**Bioaccumulation**
Confidential Brominated Polymer	Confidential	***L***	***L*¤**	**L**	***L*¤**	***L*¤**	***L*¤**	***L*¤**	***L***	***L***	**L**	**VL**	***L***	***M*^{T}¤**	**VH** ^{T}	***M*^{T}¤**

Confidential Brominated Polymer

	CASRN: Confidential CASRN
	MW: >1,000
	MF: Confidential MF
	Physical Forms: **Neat:** Solid
	Use: Flame retardant
SMILES: Confidential SMILES notation; not amenable to the generation of a SMILES notation	
Synonyms: Emerald Innovation 1000™	
Chemical Considerations: This material was assessed using guidance from HPV and Sustainable Futures criteria and by analysis of confidential materials with similar structures, substituents, and molecular weights, in the absence of experimental values (EPA, 1999; EPA, 2011). Impurities have been found in analogous substances and could potentially be present in this substance. A summary of the hazard designations for the impurities are provided in the hazard summary table. This chemical is subject to testing for the bioaccumulation and chronic aquatic toxicity endpoints. Testing for the presence of these impurities is required under consent order.	
Polymeric: No **Oligomers:** Not applicable	
Metabolites, Degradates and Transformation Products: None	
Analog: None **Endpoint(s) using analog values:** Not applicable	**Analog Structure:** Not applicable
Structural Alerts: None identified	
Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2012).	
Hazard and Risk Assessments: None identified	
U.S. EPA TSCA Regulatory Status: This chemical is not listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.	

Confidential Brominated Polymer			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	270-329 (Measured) According to an OECD guideline study.	Submitted confidential study	Adequate, OECD guideline study.
	>180 (Measured) According to OECD Guideline 102	Submitted confidential study	Adequate, OECD guideline study.
Boiling Point (°C)	>300 (Estimated)	Professional judgment; EPA, 1999	Cutoff value used for large, high MW solid.
	>400 (Measured) According to OECD Guideline 103	Submitted confidential study	Cutoff value obtained from guideline study.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2011	Cutoff value for nonvolatile compounds according to SF assessment guidance.
	$<1.5x10^{-6}$ (Measured) According to OECD Guideline 104	Submitted confidential study	Cutoff value obtained from guideline study.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	Professional judgment; EPA, 1999	Cutoff value for nonsoluble compounds according to HPV assessment guidance.
	<0.1 (Measured) According to OECD Guideline 105	Submitted confidential study	Cutoff value obtained from guideline study.
Log K_{ow}	>10 (Estimated)	Professional judgment; EPA, 2011	Cutoff value used according to SF assessment guidance.
	>9 (Measured) According to HPLC Method for OECD Guideline Method 117	Submitted confidential study	Cutoff value obtained from guideline study.
Flammability (Flash Point)	Not highly flammable (Measured) According to Method A10 Flammability (Solids) of Commission Regulation (EC) No 440/2008	Submitted confidential study	Adequate, guideline studies.

Confidential Brominated Polymer			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	No relative self-ignition temperature below its melting temperature (Measured) According to a study comparable to method A16 Relative Self-Ignition Temperature for Solids of Commission Regulation (EC) No 44012008	Submitted confidential study	
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	7 (Measured)	Submitted confidential study	This material does not contain any function groups that are anticipated to ionize in solution.
pK_a	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.

Confidential Brominated Polymer				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**No absorption is expected for any route of exposure. This substance is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body. No data located.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No absorption is expected for all routes of exposure based on physical/chemical properties (Estimated)	Professional judgment	Professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
Acute Mammalian Toxicity		**LOW: This material has a MW >1,000 and limited water solubility. It is expected to have limited bioavailability and therefore is of low potential for acute mammalian toxicity. No experimental data located.**		
Acute Lethality	**Oral**	Limited bioavailability expected (Estimated)	Professional judgment	Professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
	Dermal			
	Inhalation			
Carcinogenicity		**LOW: This material has a MW >1,000 and limited water solubility. It is expected to have limited bioavailability and few to no low MW components. Additionally, no crosslinking, swellability, dispersability, reactive functional groups, potential for inhalation, or hindered amine groups are expected and therefore this chemical has a low potential for carcinogenicity. No experimental data located.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)	Limited bioavailability expected (Estimated)	Professional judgment	Professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
	Combined Chronic Toxicity/ Carcinogenicity			
Genotoxicity		**LOW: This material did not cause gene mutations in bacteria or chromosomal aberrations in human lymphocyte cells *in vitro*. In addition, this material has a MW >1,000 and limited water solubility. It is expected to have limited bioavailability and therefore is of low potential for genotoxicity.**		

Confidential Brominated Polymer				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Gene Mutation *in vitro*	Negative, Ames assay of *Salmonella typhimurium* strains TA98, TA100, TA1535, TA1537 and *Escherichia coli* WP2 *uvrA* both with and without metabolic activation.	Submitted confidential study	Study conducted according to OECD test guideline 471.Test substance purity: 100%.
	Gene Mutation *in vivo*	Limited bioavailability expected (Estimated)	Professional judgment	Based on professional judgment based on the analysis of confidential materials with similar structures, substituents, and molecular weight.
	Chromosomal Aberrations *in vitro*	Negative for chromosomal aberrations in human lymphocytes both with and without metabolic activation.	Submitted confidential study	Study conducted according to OECD test guideline 473. Test substance purity: 100%.
	Chromosomal Aberrations *in vivo*	Limited bioavailability expected (Estimated)	Professional judgment	Based on professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
	DNA Damage and Repair			No data located.
	Other			No data located.
Reproductive Effects		**LOW: This material has a MW >1,000 and limited water solubility. It is expected to have limited bioavailability and therefore is of low potential for reproductive toxicity. No experimental data located.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment	Based on professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			

Confidential Brominated Polymer				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**LOW: This material has a MW >1,000 and limited water solubility. It is expected to have limited bioavailability and therefore is of low potential for developmental toxicity. No experimental data located.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment	Based on professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			
	Postnatal Development			
Neurotoxicity		**LOW: This material has a MW >1,000 and limited water solubility. It is expected to have limited bioavailability and therefore is of low potential for neurotoxicity. No experimental data were located.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment	Based on professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
Repeated Dose Effects		**LOW: This material has a MW >1,000 and limited water solubility. It is expected to have limited bioavailability and therefore is of low potential for repeated dose toxicity. No experimental data located.**		
		Limited bioavailability expected (Estimated)	Professional judgment	Based on professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
Skin Sensitization		**LOW: Estimated to have low potential for skin sensitization based on expert judgment.**		
Skin Sensitization		Low potential for skin sensitization (Estimated)	Expert judgment	Based on professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
Respiratory Sensitization		**LOW: Estimated to have low potential for respiratory sensitization based on expert judgment.**		

Confidential Brominated Polymer				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Respiratory Sensitization		Low potential for skin sensitization (Estimated)	Expert judgment	Based on professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
Eye Irritation		**LOW: This material was a minimal eye irritant in rabbits.**		
	Eye Irritation	Minimally irritating in rabbits; clearing within 24hours.	Submitted confidential study	Study conducted according to OECD test guideline 405. Test substance purity: 100%.
Dermal Irritation		**VERY LOW: This material was not a skin irritant in rabbits.**		
	Dermal Irritation	No evidence of skin irritation in rabbits.	Submitted confidential study	Study conducted according to OECD test guideline 404; single 4-hour, semi-occluded application to intact skin. Test substance purity: 100%.
Endocrine Activity		**No data located. This material has a MW >1,000 and limited water solubility. It is not expected to have endocrine activity due to its poor bioavailability and inability to readily metabolize in the body.**		
		Limited bioavailability expected (Estimated)	Professional judgment	Based on professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
Immunotoxicity		**This material has a MW >1,000 and limited water solubility. It is expected to have limited bioavailability and therefore is of low potential for immunotoxicity. No experimental data located.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment	Based on professional judgment based on the analysis of confidential materials with similar structures, substituents, and MW.
ECOTOXICITY				
ECOSAR Class		Not applicable		

Confidential Brominated Polymer			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Acute Toxicity	**LOW: Non-ionic solids with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW components are estimated to display no effects at saturation. These solids display no effects at saturation because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low concern for those materials that display no effects at saturation.**		
Fish LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity	**MODERATE: Test data regarding chronic aquatic toxicity were not located on this substance therefore potential for hazard is uncertain. EPA has predicted the behavior of this substance in the environment based upon physical-chemical properties and data on structurally similar chemicals. To enable a reasoned evaluation of the environmental effects and potential degradation products, EPA requires the manufacturer to provide test data on this substance using the OECD 231 test guideline for amphibian metamorphosis 24 months from commencement of manufacture or prior to a confidential production volume trigger, whichever comes later.** **In addition, the notice of commencement for this substance includes pended testing for fish early life stage toxicity, chronic daphnia toxicity and algal toxicity (OPPTS 850.1400, 850.1300 and 850.5400 respectively). Pended testing must be submitted only if the manufacturer wishes to be released from a Consent Order.**		
Fish ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.

Confidential Brominated Polymer				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Green Algae ChV		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that this substance is anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of $<10^{-8}$ atm-m^3/mole indicates that it is not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that it is not anticipated to migrate from soil into groundwater and also has the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment	Cutoff value for nonvolatile compounds.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	EPA, 2011; Professional judgment	Cutoff value for nonmobile compounds according to SF assessment guidance.
		$\log K_{oc}$ >5 (Experimental) According to OECD Guideline 121	Submitted confidential study	Cutoff value obtained from guideline study.
	Level III Fugacity Model			No data located.

Confidential Brominated Polymer				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Persistence		**VERY HIGH: This substance has a MW >1,000. It is expected to have negligible water solubility and poor bioavailability to microorganisms indicating that biodegradation is not expected to be an important removal processes in the environment. One experimental biodegradation test using activated sludge resulted in no degradation after 28 days. Estimated hydrolysis half-lives of >1 year indicate that this will not be an important environmental removal process. Although photodegradation of brominated aromatic compounds has been observed, this process is not anticipated to lead to ultimate removal of the material. As a result, a half-life for this high MW solid is expected to be >180 days.** **While test data from environmental fate studies were not located on this substance, EPA has predicted its behavior in the environment based upon physical-chemical properties and data on structurally similar chemicals. To enable a reasoned evaluation of the human health and environmental effects of the PMN substance and potential degradation products, EPA requires the manufacturer to provide test data on this substance using the OPPTS 835.4400 test guideline on anaerobic metabolism in aquatic sediment 24 months from commencement of manufacture or prior to a confidential production volume whichever comes later.**		
Water	**Aerobic Biodegradation**	Not readily degradable (Measured) 0% degraded/BOD after 28 days; activated sludge ready biodegradability test Using a Method Relating to New Chemical Substances - Biodegradability Test of Chemical Substances by Microorganisms	Submitted confidential study	Study performed according to a standardized method.
		Recalcitrant (Estimated)	Professional judgment	High MW solids are expected to be non-biodegradable due to their limited bioavailability.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law constant.

Confidential Brominated Polymer				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Soil	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment	High MW solids are expected to be nonbiodegradable due to their limited bioavailability.
	Anaerobic Biodegradation	Recalcitrant (Estimated)	Professional judgment	High MW solids are expected to be resistant to removal under anoxic conditions biodegradable due to their limited bioavailability.
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	Not a significant fate process (Estimated)	Professional judgment	This chemical is expected to exist in the particulate phase in the atmosphere.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Professional judgment	The bromine substituent is susceptible to photolysis however; this is expected to be a relatively slow process and is not anticipated to lead to ultimate removal of the material.
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.

Confidential Brominated Polymer				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Environmental Half-Life		>180 days (Estimated)	Professional judgment	The substance has a MW greater than 1,000 and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to be readily removed by other degradative processes under environmental conditions because of limited water solubility and lack of reactive functional groups.
Bioaccumulation		**MODERATE: The bioaccumulation designation for this compound is based upon physical-chemical properties and by analogy to structurally similar chemicals. This substance is large and insoluble in water. As test data regarding bioaccumulation were not located on this substance, the potential for bioconcentration or bioaccumulation is uncertain. To enable a reasoned evaluation of the human health and environmental effects of the PMN substance and potential degradation products, EPA requires the manufacturer to provide test data on this substance using the OECD 305 test guideline for bioaccumulation in fish with dietary exposure, 36 months from commencement of manufacture or prior to attaining a confidential production volume whichever comes later.**		
	Fish BCF	<100 (Estimated)	Professional judgment	The substance has a MW >1,000 and is not anticipated to be assimilated by aquatic organisms; therefore, bioconcentration is not expected.
	BAF	<1000 (Estimated by analogy)	Professional judgment	This compound is outside the MW domain of the corresponding EPI models. The BAF estimate was based on analogy to a structurally similar confidential analog that has a Moderate hazard designation.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		

Confidential Brominated Polymer			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Ecological Biomonitoring	No data located.		
Human Biomonitoring	This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

CDC (Centers for Disease Control and Prevention). *Fourth national report on human exposure to environmental chemicals, updated tables*. Department of Health and Human Services. **2011.** http://www.cdc.gov/exposurereport/pdf/Updated_Tables.pdf (accessed on January 16, 2112).

ESIS (European chemical Substances Information System) Classification, labeling and packaging of dangerous substances annex VI to Regulation (EC) No 1272/2008 [Online] http://esis.jrc.ec.europa.eu/index.php?PGM=cla (accessed on accessed on January 16, 2112).

U.S. EPA (Environmental Protection Agency) Sustainable Futures. *Using NonCancer Screening within the SF Initiative.* Environmental Protection Agency: Washington D.C. http://www.epa.gov/opptintr/sf/pubs/noncan-screen.htm#systemic (accessed on January 16, 2112).

U.S. EPA (Environmental Protection Agency). High Production Volume (HPV) Challenge. *Determining the Adequacy of Existing Data*. U.S. Environmental Protection Agency: Washington D.C. **1999**. http://www.epa.gov/hpv/pubs/general/datadfin.htm

U.S. EPA (Environmental Protection Agency). Sustainable Futures Summary Assessment. *Interpretive Assistance Document for Assessment of Polymers.* U.S. Environmental Protection Agency: Washington D.C. **2010a.** http://www.epa.gov/oppt/sf/pubs/iad_polymers_042010.pdf as of September 2, 2011.

U.S. EPA (Environmental Protection Agency). Sustainable Futures Summary Assessment. *Assessment of Discrete Organic Chemicals*. U.S. Environmental Protection Agency: Washington D.C. **2011.** http://www.epa.gov/oppt/sf/pubs/iad_discretes_092011.pdf

U.S. EPA (Environmental Protection Agency). TSCA New Chemicals Program (NCP) Chemical Categories. U.S. Environmental Protection Agency: Washington D.C. **2010b**. http://www.epa.gov/oppt/newchems/pubs/npcchemicalcategories.pdf (accessed on Sept. 8, 2011).

Decabromodiphenyl Ethane

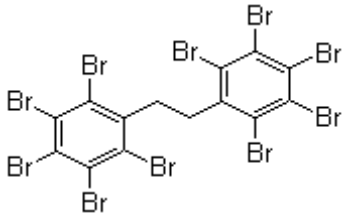
Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.
§ Based on analogy to experimental data for a structural similar compound.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Decabromodiphenyl Ethane	84852-53-9	L	*M*§	L	L	VL	*H*§	L	L		VL	VL	L	*L*	VH	*H*

Decabromodiphenyl Ethane



CASRN: 84852-53-9

MW: 971.2

MF: $C_{14}H_4Br_{10}$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: c1(Br)c(Br)c(Br)c(Br)c(Br)c1CCc1c(Br)c(Br)c(Br)c(Br)c1Br

Synonyms: Benzene, 1,1'-(1,2-ethanediyl)bis[2,3,4,5,6-pentabromo-] (TSCA Inventory); Ethane 1,2-(bispentabromophenyl); EBP; Bis(pentabromophenyl) ethane; 1,1'-(ethane-1,2-diyl)bis[pentabromobenzene]; Decabromodiphenyl ethane; DBDP-Ethane; DBDPE; Saytex 8010; Firemaster 2100

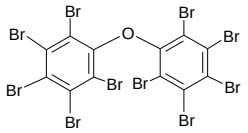
Chemical Considerations: This is a discrete organic chemical with a MW below 1000. EPI v 4.0 was used to estimate physical/chemical and environmental fate values due to an absence of experimental data. Measured values from experimental studies were incorporated into the estimations.

Polymeric: No
Oligomers: Not applicable

Metabolites, Degradates and Transformation Products: Lower brominated congeners

Analog: Decabromodiphenyl ether, confidential analogs
Endpoint(s) using analog values: Carcinogenicity; Neurotoxicity, Absorption, distribution, metabolism & excretion

Analog Structure:



Decabromodiphenyl ether
(1163-19-5)

Structural Alerts: Immunotoxicity, polyhalogenated aromatic hydrocarbons (U.S. EPA, 2011); test data are available to address this category.

Risk Phrases: Not classified by Annex I Directive 67/548/EEC & IUCLID (Pakalin et al., 2007)

Hazard and Risk Assessments: An environmental risk evaluation report was completed by the UK government Environment Agency (Dungey et al., 2007)

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory and is a commenced Premanufacture Notice substance. It was subject to a Consent Order that contained a Significant New Use Rule regulating the chemical as follows: this product cannot be released into U.S. waters. This requirement does not apply once the flame retardant substance has been incorporated into a resin.

Decabromodiphenyl Ethane CASRN 84852-53-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	350 (Measured)	Mack, 2004	Adequate.
Boiling Point (°C)	>350 (Estimated)	Professional judgment	Based on the reported experimental melting point value.
Vapor Pressure (mm Hg)	$<7.5 \times 10^{-7}$ (Measured)	Hardy, 2004	Adequate.
Water Solubility (mg/L)	7.2×10^{-4} (Measured)	Hardy, 2004	Adequate.
Log K_{ow}	>10 (Estimated)	EPI; EPA, 2011	Cutoff value used according to SF assessment guidance.
	3.55 According to column elution method OPPTS 830.7560. The concentration in the water phase was very close to the measured water solubility it was noted that a higher stock solution concentration could have led to a higher K_{OW} value using this technique. (Measured)	Dungey et al., 2007	The value was reported in a secondary source and was obtained using a guideline study however, it is considered unreliable based on comparison to other substances that contain multiple bromine atoms.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.

Decabromodiphenyl Ethane CASRN 84852-53-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Decabromodiphenyl ethane, as a neat material, is estimated to not be absorbed through the skin and have poor skin absorption when in solution. Decabromodiphenyl ethane is expected to have poor absorption via the lungs and gastrointestinal (GI) tract. Decabromodiphenyl ethane is poorly absorbed in the GI tract following oral exposure and is mainly excreted in the feces. If absorption does occur, decabromodiphenyl ethane is distributed to the serum, liver, kidney, and adipose tissues and undergoes biotransformation to form metabolites.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	Not absorbed through the skin as the neat material; poor absorption through skin if in solution; poor absorption from the lung and GI tract. (Estimated by analogy)	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/chemical properties.
		In an acute (single dose) oral study in rats, decabromodiphenyl ethane was poorly absorbed (if at all) in the GI tract and was excreted in the feces. There were no detectable levels of decabromodiphenyl ethane in bile, blood or urine. This finding is consistent with the poor solubility and the MW of decabromodiphenyl ethane.	Hardy, 2004	Guideline study (performed according to GLP, reported in a secondary source; test substance: Saytex 8010.
		Rats, 90-day oral exposure; decabromodiphenyl ethane was found to be distributed to the tissues examined (serum, liver, kidney, and adipose); biotransformation occurred in rats, though debromination to lower brominated bromodiphenyl ethanes was not the primary metabolic pathway; proposed metabolites were identified as $MeSO_2$-nona-BDPE and $EtSO_2$-nona BDPE.	Wang et al. 2010	There was an absence of measurable radioactivity in samples taken during study that suggest decabromodiphenyl ethane is poorly absorbed by the oral route.

Decabromodiphenyl Ethane CASRN 84852-53-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Acute Mammalian Toxicity		**LOW: Based on a rat oral LD_{50} of >5,000 mg/kg and a rabbit dermal LD_{50} of >2,000 mg/kg. No acute inhalation hazard data located.**		
Acute Lethality	**Oral**	Rat oral LD_{50} >5,000 mg/kg	Hardy et al. 2002; Hardy, 2004	Guideline study; test substance: Saytex 8010.
	Dermal	Rabbit dermal LD_{50} >2,000 mg/kg	Hardy et al. 2002; Hardy, 2004	Guideline study, reported in a secondary source; test substance: Saytex 8010.
	Inhalation			No data located.
Carcinogenicity		**MODERATE: Potential for carcinogenicity based on analogy to decabromodiphenyl ether and professional judgment. No experimental carcinogenicity data for exposure to decabromodiphenyl ethane located.**		
	OncoLogic Results			Structure could not be evaluated by OncoLogic.
	Carcinogenicity (Rat and Mouse)	Potential for carcinogenicity; increased incidence of neoplastic nodules of the liver in rats; equivocal evidence of increased incidences of hepatocellular adenomas or carcinomas and thyroid gland follicular cell adenomas or carcinomas in male mice. (Estimated by analogy)	Professional judgment	Estimated based on the high potential for bioaccumulation and by analogy to decabromodiphenyl ether which resulted in potential carcinogenic effects following chronic exposure in a NTP study.
	Combined Chronic Toxicity/ Carcinogenicity			No data located.

Decabromodiphenyl Ethane CASRN 84852-53-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Genotoxicity		**LOW: Based on negative experimental results for gene mutations in *Salmonella* and chromosomal aberrations in Chinese hamster ovary (CHO) cells.**		
	Gene Mutation *in vitro*	Negative for gene mutations in *Salmonella typhimurium* strains TA98, TA100, TA1535, TA1537 and *Escherichia coli* WP2 uvrA with and without exogenous metabolic activation.	Hardy et al. 2002; Hardy, 2004	Guideline study (according to Japanese MITI and GLP guidelines), reported in a secondary source; test substance: Saytex 8010.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	Negative for chromosomal aberrations in CHO cells with and without metabolic activation.	Hardy et al. 2002; Hardy, 2004	Guideline study (according to Japanese MITI and GLP guidelines), reported in a secondary source; test substance: Saytex 8010.
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: The located data suggest no reproductive effects based on a NOEL for maternal and fetal toxicity of ≥1,250 mg/kg/day in rats and rabbits. However, there is uncertainty in this hazard designation because the exposure was of subchronic (gestational) duration and the studies were not experimentally designed as a reproduction toxicity screen or combined repeated dose/reproduction/developmental toxicity screen.**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.

Decabromodiphenyl Ethane CASRN 84852-53-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Reproduction and Fertility Effects	There was no evidence of treatment-related adverse effects on the reproductive system in two developmental toxicity studies in rats and rabbits. NOEL (maternal and fetal) ≥1,250 mg/kg/day (highest dose tested) LOEL: not established	Hardy, 2004, Hardy et al., 2010	Guideline study (according to US TSCA Guidelines and GLP) reported in a secondary source; test substance: Saytex 8010.
Developmental Effects		**VERY LOW: There were no maternal or fetal toxicity effects in rats or rabbits exposed during gestation to doses up to 1,250 mg/kg/day.**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Prenatal Development	In two developmental oral gavage studies in mated female rats (GD 6-15) and rabbits (GD 6-18), there were no treatment-related fetal malformations or developmental variations. No maternal toxicity was evident. NOEL (maternal and fetal) ≥1,250 mg/kg/day (highest dose tested) LOEL: Not established	Hardy et al. 2002; Hardy, 2004; Hardy et al. 2010	Guideline study (according to US TSCA Guidelines and GLP) reported in a secondary source; test substance: Saytex 8010.
	Postnatal Development			No data located.
Neurotoxicity		**HIGH: Estimated to have potential for neurobehavioral effects based on analogy to decabromodiphenyl ether and professional judgment.**		
	Neurotoxicity Screening Battery (Adult)	Mice as neonates (day 3, 10, 19), single oral dose; neurobehavioral effects. (Estimated by analogy)	Professional judgment	Estimated based on analogy to decabromodiphenyl ether.

Decabromodiphenyl Ethane CASRN 84852-53-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects	**LOW: Based on a NOAEL and LOAEL of ≥1,000 mg/kg/day in 28 and 90-day oral rat studies, respectively. Experimental data for decabromodiphenyl ethane reported increased liver weights associated with minimal and transient hepatocellular vacuolization following a 90-day oral exposure. The increase in liver weights was associated with minimal to slight hepatocellular vacuolation, which had no long-term effect and was resolved after a 28-day recovery period at the highest doses tested (1,000 mg/kg/day). A LOAEL was not established in the 28-day study, as the highest doses tested did not produce adverse effects. By analogy to decabromodiphenyl ether and with the potential for bioaccumulation, there is potential for expression of adverse effects in longer term studies.**		
	In a 28-day oral gavage study in rats, there was no mortality or clinical signs of toxicity, and no treatment-related statistically significant effects for changes in body weight, food consumption, body weight gain, hematology, serum chemistry, urinalysis, gross necropsy, relative and absolute organ weight, or histopathology. NOAEL >1,250 mg/kg/day (highest dose tested) LOAEL: not established	Hardy, 2004	Guideline study (according to US TSCA Guidelines and GLP), reported in a secondary source Organisation for Economic Cooperation and Development (OECD) 407; test substance: Saytex 8010.

Decabromodiphenyl Ethane CASRN 84852-53-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	In a 90-day oral gavage study in rats, there was no mortality, clinical or systemic signs of toxicity or ocular lesions; no changes in urine or serum chemistry, hematology, body weight, body weight gain or food consumption. Mean liver weights increased in males at the highest dose tested (but not at lower doses). Increased liver weight was associated with minimal to slight hepatocellular vacuolation and minimal to slight centrilobular hepatocytomegaly; liver changes returned to normal after a 28-day recovery period; no changes in female rat livers. NOAEL ≥ 320 mg/kg/day LOAEL = 1,000 mg/kg/day (highest dose tested)	Hardy et al. 2002; Hardy, 2004	Guideline study(according to US TSCA Guidelines and GLP), reported in a secondary source; OECD 408; test substance: Saytex 8010.
	In a 90-day oral study in rats, there were no significant changes in body weight, or absolute and relative liver and kidney weights; hepatotoxicity indicated by changes in serum chemistry including Increased TBA levels, decreased Cr, AST, and ALP activities; increased serum T3 thyroid hormone levels; increased CYP3A2 mRNA expression. LOAEL = 100 mg/kg/day (only dose tested)	Wang et al. 2010	Only one dose tested; a NOAEL was not established; no histopathological assessments were made on the liver; data are insufficient to determine a hazard designation for this endpoint.

Decabromodiphenyl Ethane CASRN 84852-53-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Skin Sensitization		**LOW: Experimental data for decabromodiphenyl ethane was negative for skin sensitization in the guinea pig.**		
	Skin Sensitization	Negative for skin sensitization, guinea pigs	Hardy et al. 2002; Hardy, 2004	Guideline study, reported in a secondary source; test substance: Saytex 8010.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**VERY LOW: Decabromodiphenyl ethane is not an eye irritant in rabbits.**		
	Eye Irritation	Non-irritant, rabbit	Hardy et al. 2002; Hardy, 2004	Guideline study, reported in a secondary source; test substance: Saytex 8010.
Dermal Irritation		**VERY LOW: Decabromodiphenyl ethane is not a skin irritant in rabbits.**		
	Dermal Irritation	Non-irritant, rabbit	Hardy et al. 2002; Hardy, 2004	Guideline study, reported in a secondary source; test substance: Saytex 8010.
Endocrine Activity		**There were limited data located for this endpoint.**		
		90-day oral study in rats; increased serum T3 thyroid hormone levels; no effects on thyroxine levels	Wang et al. 2010	Only one dose tested; a NOAEL was not established, so it is uncertain where effects would occur; did not evaluate thyroid weight, or histopathology.
Immunotoxicity		**There were no immunotoxicity effects noted in a 90-day oral gavage study in rats.**		
	Immune System Effects	There were no immunotoxicity effects, noted in a 90-day oral gavage study in rats.	Hardy et al. 2002; Hardy, 2004	Guideline study(according to US TSCA Guidelines and GLP), reported in a secondary source; OECD 408; test substance: Saytex 8010.

Decabromodiphenyl Ethane CASRN 84852-53-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
ECOTOXICITY			
ECOSAR Class			
Acute Toxicity	**LOW: Experimental values for daphnia and fish, and ECOSAR estimations for green algae and saltwater invertebrate suggest that decabromodiphenyl ethane exhibits no effects at saturation (NES) and is not acutely toxic to fish, daphnia or green algae**		
Fish LC_{50}	Rainbow trout (*Oncorhynchus mykiss*) 96-hour LLR_{50} >110 mg/L (static, nominal)	Hardy, 2004	The reported value was determined using a water accommodated fraction (WAF). According to OECD guidelines, WAFs should only be used to determine toxicity of multi-component substances. As a result, the reported value is greater than this material's water solubility.
	Fish 96-hour LC_{50} = 4.29E-008 mg/L ECOSAR: Neutral Organics (Estimated)	EPI	NES: The log K_{ow} of 13.64 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.

Decabromodiphenyl Ethane CASRN 84852-53-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Daphnid LC_{50}	Daphnia (*Daphnia magna*) 48-hour LLR_{50} >110 mg/L (static, nominal)	Hardy, 2004	The reported value was determined using a WAF. According to OECD guidelines, WAFs should only be used to determine toxicity of multi-component substances. As a result, the reported value is greater than this material's water solubility.
	Daphnia (*Daphnia magna*) 48-hour EC_{50} = 19 µg/L (0.019 mg/L, nominal)	Nakari and Huhtala, 2010	Although in a guideline study (ISO 6341, 1996), the reported value is greater than the substance's water solubility (0.72 µg/L).
	Daphnia 48-hour LC_{50} = $1.35x10^{-7}$ mg/L ECOSAR: Neutral Organics (Estimated)	EPI	NES: The log K_{ow} of 13.64 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
Saltwater Invertebrate LC_{50}	Mysid Shrimp 96-hour LC_{50} = 28 mg/L ECOSAR: Neutral Organics (Estimated)	EPI	NES: The log K_{ow} of 13.64 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
Green Algae EC_{50}	Green Algae (*Psuedokirchneriella subcapitata)* 96-hour EL_{50} and NOAEL >110 mg/L (static, nominal)	Hardy, 2004	The reported value was determined using a WAF. According to OECD guidelines, WAFs should only be used to determine toxicity of multi-component substances. As a result, the reported value is greater than this material's water solubility.
	Green Algae 96-hour EC_{50} = $1.01x10^{-5}$ mg/L ECOSAR: Neutral Organics (Estimated)	EPI	NES: The log K_{ow} of 13.64 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.

Decabromodiphenyl Ethane CASRN 84852-53-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Chronic Aquatic Toxicity	**LOW: Estimated data suggest NES for chronic aquatic toxicity endpoints.**		
Fish Chronic Value (ChV)	Zebra fish (*Danio rerio*) static-renewal (48-hr renewal intervals) egg-larvae test: LOEC = 12.5 µg/L (0.0125 mg/L, nominal) based on mortality of eggs and hatched larvae; NOEC < 12.5 µg/L (0.0125 mg/L, nominal)	Nakari and Huhtala, 2010	Not a standard test for the determination of hazard for which emphasis is strongly placed on whole organism studies; Supporting information presented in a non-standard, guideline study (ISO 12890, 1999) with insufficient study details. The solvent dimethyl sulfoxide was used to solubilize test substance into solution. Non-standard dilution water was used. Test concentrations were above the identified water solubility value (0.72 µg/L).
	Fish 30-day ChV = $9.76x10^{-9}$ mg/L ECOSAR: Neutral Organics (Estimated)	EPI	NES: The log K_{ow} of 13.64 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
Daphnid ChV	Daphnid ChV = $9. 91x10^{-8}$ mg/L ECOSAR: Neutral Organics (Estimated)	EPI	NES: The log K_{ow} of 13.64 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.

Decabromodiphenyl Ethane CASRN 84852-53-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Saltwater Invertebrate ChV	Mysid Shrimp ChV = $2.91x10^{-14}$ mg/L ECOSAR: Neutral Organics (Estimated)	EPI	NES: The log K_{ow} of 13.64 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
Green Algae ChV	Green Algae ChV = $2.68x10^{-5}$ mg/L (ECOSAR Estimate, Class: Neutral Organics (Estimated)	EPI	NES: The log K_{ow} of 13.64 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
Sediment Dwelling Organisms ChV	Midge (*Chironmus riparius*) 28-day NOEC = 5,000 mg/kg dry sediment (highest concentration tested)	Hardy, 2004	Adequate, guideline study (according to OECD, OPPTS and GLP) although full study details not available.
	Oligochaete (*Lumbriculus variegates*) 28-day NOEC = 5,000 mg/kg dry sediment (highest concentration tested)	Hardy, 2004	Adequate, guideline study (according to OECD, OPPTS and GLP) although full study details not available.
Earthworm Subchronic Toxicity	Earthworm 28-day survival and reproduction test: NOEC (survival) = 3,720 mg/kg dry soil (highest dose tested); LOEC (reproduction) = 3720 mg/kg dry soil; NOEC (reproduction) = 1,910 mg/kg dry soil	Hardy, 2004	Adequate, guideline study (according to OECD, OPPTS and GLP) although full study details not available.

Decabromodiphenyl Ethane CASRN 84852-53-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**Based on the Level III fugacity models incorporating the located experimental property data, decabromodiphenyl ethane is expected to partition primarily to soil. Decabromodiphenyl ethane is expected to be immobile in soil based on its estimated K_{oc}. Leaching of decabromodiphenyl ethane through soil to groundwater is not expected to be an important transport mechanism. Estimated volatilization half-lives indicate that it will be non-volatile from surface water. Volatilization from dry surface is also not expected based on its vapor pressure. In the atmosphere, decabromodiphenyl ethane is expected to exist solely in the particulate phase, based on its estimated vapor pressure. Particulates may be removed from air by wet or dry deposition.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	EPI; Professional judgment	Cutoff value for non volatile compounds based on the ionic nature of the material.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	EPI; EPA, 2011	Cutoff value for non mobile compounds according to SF assessment guidance.
	Level III Fugacity Model	Air = <1% Water = 4.5% Soil = 95% Sediment = <1% (Estimated)	EPI	
Persistence		**VERY HIGH: Very high persistence of decabromodiphenyl ethane is expected based on experimental biodegradation data. Decabromodiphenyl ethane was determined to not be readily biodegradable in a 28-day MITI test nor was it inherently degradable in a 90-day aerobic sewage/soil test using pre-exposed innocula. Decabromodiphenyl ethane is not expected to undergo hydrolysis since it does not contain hydrolysable functional groups. The atmospheric half-life of decabromodiphenyl ethane is estimated to be 4.5 days, although it is expected to exist primarily in the particulate phase in air. Laboratory studies have demonstrated photolysis of decabromodiphenyl ethane, although the rate of this process under environmental conditions has not been established.**		

Decabromodiphenyl Ethane CASRN 84852-53-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Water	**Aerobic Biodegradation**	Not inherently biodegradable according to OECD, 2000 guideline study (Measured). The decabromodiphenyl ethane treated bottles evolved an amount of the theoretical inorganic carbon (ThIC) equivalent to that of the untreated controls. Transformation of [^{14}C]-labeled decabromodiphenyl ethane was not observed in the 90-d aerobic study	Hardy, 2011	Adequate, guideline study.
		Not readily biodegradable by activated sewage sludge over 28 days (Japanese MITI/OECD 301C Modified MITI) (Measured)	Hardy, 2004	Adequate, guideline study.
	Volatilization Half-life for Model River	>1 year (Estimated)	EPI	
	Volatilization Half-life for Model Lake	>1 year (Estimated)	EPI	
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation	Probable (Anaerobic-methanogenic biodegradation probability model)	EPI	
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	4.5 days (Estimated)	EPI	

Decabromodiphenyl Ethane CASRN 84852-53-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Reactivity	**Photolysis**	Debrominated congeners identified by a photolytic degradation with a 125W high-pressure mercury lamp experiment using GC/EI-MS and GC/ECNIMS analysis. (Measured)	Wang et al. 2010	Non guideline study that demonstrates the potential for both direct and indirect photolysis in the environment. The significance of the laboratory removal rates under environmental conditions cannot be determined.
	Hydrolysis	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to hydrolyze readily under environmental conditions.
Environmental Half-Life		>1 year (Estimated)	EPI	Half-life estimated for the predominant compartment, as determined by EPI and the PBT Profiler methodology.
Bioaccumulation		**HIGH: Monitoring data suggest that decabromodiphenyl ethane may bioaccumulate in aquatic and terrestrial species. Two experimental BCF values are less than the low criteria cutoff of 100 indicating that bioaccumulation may be low in fish.**		
	Fish BCF	<2.5 at a concentration of 0.5 mg/L after 8 weeks in carp (*Cyprnus carpio*) (Measured)	Hardy, 2004	Adequate.
		<25 at a concentration of 0.05 mg/L after 8 weeks in carp (*Cyprnus carpio*) (Measured)	Hardy, 2004	Adequate.
	BAF	62 (Estimated)	EPI	
	Metabolism in Fish			No data located.

Decabromodiphenyl Ethane CASRN 84852-53-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL MONITORING AND BIOMONITORING			
Environmental Monitoring	Decabromodiphenyl ethane was reported in sludge, sediment, and collected from 2001-2002 (Kierkegaard, 2004). The presence of decabromodiphenyl ethane was reported in Swedish lake sediment (Ricklund et al., 2010). The presence of decabromodiphenyl ethane in sludge from countries worldwide (Ricklund et al., 2008). A review article by Betts (2009) refers to a number of articles reporting decabromodiphenyl ethane in the environment.		
Ecological Biomonitoring	A review article by Betts (2009) notes detections of decabromodiphenyl ethane in North American seagulls, five species of Chinese water birds, giant and red pandas from China, fish from Lake Winnipeg, and herring gull eggs.		
Human Biomonitoring	This chemical was not included in the NHANES biomonitoring report (CDC, 2011)		

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Decabromodiphenyl Ether

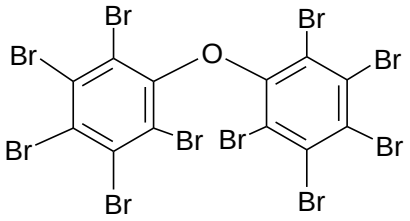
Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from estimation software and professional judgment.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Decabromodiphenyl Ether	1163-19-5	L	M	L	L	H	H	M	L		L	L	*L*	*L*	VH	*H*

Decabromodiphenyl Ether



CASRN: 1163-19-5

MW: 959.2

MF: $C_{12}Br_{10}O$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: O(c1c(c(c(c(c1Br)Br)Br)Br)Br)c1c(c(c(c(c1Br)Br)Br)Br)Br

Synonyms: Benzene, 1,1'-oxybis[2,3,4,5,6-pentabromo- (TSCA Inventory); 1,1'-Oxybis(2,3,4,5,6-pentabromobenzene); Adine 505; AFR 1021; BDE 209; BDE-209; BR 55N; Berkflam B; Bis(pentabromophenyl) ether, Bis(pentabromophenyl) oxide; Bromkal 82-0DE; Bromkal 83-10DE; Caliban F/R-P 39P; DB 10; DB 101; DB 102; Decabromodiphenyl oxide (DBDPO); DE 83; De 83R; DP 10F; Decabromodiphenyl ether; Decabrom; Decabromodiphenyl oxide; Decabromobiphenyl ether; Decabromobiphenyl oxide;EB 10; EB 10FP; EB 10W; EB 10WS; EBR 700; F/R-P 53; Fire Cut 83D; Flame Cut 110R; Flame Cut Br 100; FR 10; FR 300; FR 300BA; FR-PE; FR-PE(H); FRP 53; Nonnen DP 10; Nonnen DP 10(F); PBED 209; Planelon DB; Planelon DB 100; Planelon DB 101; Plasafety EB 10; Plasafety EBR 700; Saytex 102; Saytex 102E; Tardex 100

Chemical Considerations: This is a discrete organic chemical with a MW below 1000. EPI v 4.0 was used to estimate physical/chemical and environmental fate values in the absence of experimental data. Measured values from experimental studies were incorporated into the estimations.

Polymeric: No **Oligomers:** Not applicable	
Metabolites, Degradates and Transformation Products: Lower brominated diphenyl ether (BDE) congeners: a range of penta- to nonaBDEs (with 2,2',4,4',5,6'-hexabromodiphenyl ether being most prevalent). Polybrominated dibenzofurans (European Chemicals Bureau, 2002)	
Analog: No analog **Endpoint(s) using analog values:** Not applicable	**Analog Structure:** Not applicable
Structural Alerts: Polyhalogenated aromatic hydrocarbons, immunotoxicity (U.S. EPA 2011a)**;** test data are available to address this category.	
Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2012).	
Hazard and Risk Assessments: U.S. EPA IRIS - Toxicological Review of Decabromodiphenyl ether (2008). Assessments were prepared for decabromodiphenyl ether by the Washington Department of Ecology and Department of Health (Washington DOE, 2008), Illinois Environmental Protection Agency (Illinois EPA, 2007), Danish Environmental Protection Agency (Danish, 2007), European Chemicals Bureau (European Chemicals Bureau, 2002), German Federal Ministry of the Environment (German Federal Ministry of the Environment, 2001), and the National Academy of Sciences National Research Council (NAS, 2000). The Maine Department of Environmental Protection, Safer Alternatives Assessment for Decabromodiphenyl Ether Flame Retardant in Plastic Pallets, includes a Green Screen Assessment of decabromodiphenyl ether (Maine DEP, unpublished). Decabromodiphenyl ether was also part of the High Production Volume (HPV) Data Summary and Test Plan (U.S. EPA, 2005) and the Voluntary Childrens' Chemical Evaluation Program (VCCEP) (U.S. EPA, 2012).	
U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory and is subject to a Section 4 test rule. Decabromodiphenyl ether is part of the Polybrominated Diphenyl Ether (PBDEs) Action Plan which addresses the voluntary phase-out of manufacture and import of decabromodiphenyl ether by manufacturers in the U.S.; development of a Significant New Use Rule (SNUR) and combined Section 4 test rule where the significant new use would be manufacture, (including import) of decabromodiphenyl ether or articles to which decabromodiphenyl ether has been added; and the addition of commercial PBDE mixtures and/or the congeners they contain to the Concern List under TSCA section 5(b)(4) as chemicals that present or may present an unreasonable risk of injury to health or the environment (U.S. EPA, 2009).	

Decabromodiphenyl Ether CASRN 1163-19-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	300-310 (Measured)	European Chemicals Bureau, 2000; European Chemicals Bureau, 2002	Adequate; consistent values, which span a relatively narrow range, have been reported in a secondary sources.
	305 (Measured)	Lide, 2008	Adequate value cited from standard reference source.
	307 (Measured)	Fu and Suuberg, 2011	Adequate value obtained from differential scanning calorimeter.
Boiling Point (°C)	>320 (decomposes) (Measured)	European Chemicals Bureau, 2002	Adequate; reported in a secondary source.
Vapor Pressure (mm Hg)	3.5×10^{-8} at 21ºC (Measured) GLP Spinning Rotor Method	European Chemicals Bureau, 2002	Adequate, guideline study.
	$9.02\text{x}10^{-13}$ at 25ºC (Extrapolated) Knudsen Effusion Method	Fu and Suuberg, 2011	Adequate value for low volatility substance; obtained using an indirect measurement technique.
Water Solubility (mg/L)	$<1.00\times10^{-4}$ at 25ºC (Measured) GLP Column Elution Method Value reported was the detection limit	European Chemicals Bureau, 2002	Adequate; value reported in a secondary source.
	2×10^{-3} to 3×10^{-3} (Measured)	European Chemicals Bureau, 2000	Sufficient details were not available to assess the quality of this study reported in a secondary source.
Log K_{ow}	6.27 (Measured) GLP Generator Column Method	European Chemicals Bureau, 2002	Adequate; value reported in a secondary source.
Flammability (Flash Point)	Not flammable (Estimated)	European Chemicals Bureau, 2000	Adequate; value reported in a secondary source.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.

Decabromodiphenyl Ether CASRN 1163-19-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a	Not applicable	Professional judgment	Dissociation is not expected; the chemical does not contain ionizable functional groups.
HUMAN HEALTH EFFECTS			
Toxicokinetics	**Although experimental findings in human and animal studies suggest that decabromodiphenyl ether is poorly absorbed following oral and dermal administration, even low levels of decabromodiphenyl ether are physiologically relevant due to its chemical properties. 99% of decabromodiphenyl ether is eliminated from the body in the feces with ≤ 0.01% excreted in urine. Decabromodiphenyl ether is mainly excreted as unchanged parent compound but may also be excreted in the form of metabolites. Some conversion of parent compound may be mediated by intestinal epithelium or microflora. Monitoring studies with human volunteers demonstrate that decabromodiphenyl ether can be absorbed, distributed to mammary tissue and secreted in human breast milk during lactation.**		
Dermal Absorption *in vitro*	Female hairless mice were exposed in a flow-through diffusion cell system to carrier-free ^{14}C-labeled decabromodiphenyl ether (>98% pure) at doses of 6, 30 or 60 nmol. % absorption was determined at 6, 12, 18 and 24 hours. Most of dose was taken up within the first 6 hours and very little compound was absorbed (0.04-0.34%). Total dose retained in the skin and transported to receptor fluid was 20.5%, 3.3% and 1.9% for 6, 30 and 60 nmol doses, respectively.	EPA, 2008	Reported in a secondary source. The results of this may overestimate the amount of decabromodiphenyl ether that would be absorbed by human skin, as mouse skin has been found to be more permeable to several chemicals.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		F344/N male rats fed 238 to 51,000 ppm unlabeled DBDPO (97.9-99.2% pure) in the diet on days 1-7 and ^{14}C DBDPO on day 8. Average daily consumption estimated to be 3,718 mg/kg-day. 91.3% of radioactivity was recovered in the feces 72 hours after exposure. Recovery was not related to administered dose. Low level of radioactivity in the liver and fat (0.064% and 0.008% of dose in liver for low and high dose, respectively; 0.157 and 0.09% in fat for low and high dose, respectively)	European Chemicals Bureau, 2002	Study details reported in a secondary source.
		F344/N male rats fed 277 or 48,000 ppm unlabeled DBDPO on days 1-7 and 9-10 or 9-11 and ^{14}C DBDPO on day 8. Doses were equivalent to 22-25 and 4500-5000 mg/kg-day. 82.5% of radioactivity was recovered in feces. Recovery was not related to administered dose. Excretion in the urine was ≤ 0.01%. Trace levels of radioactivity were found in all major organs and tissues with the highest concentration found in the liver, kidney, lung, skin and adipose tissue. DBDPO and 3 main metabolites were detected in the feces. % of metabolites increased with increasing DBDPO concentration in diet, but DBDPO was primary compound eliminated.	European Chemicals Bureau, 2002	Study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Intravenous study in F344/N rats injected with 1.07 mg/kg ^{14}C DBDPO 75% of intra-venous dose was detected in feces and gut contents after 72 hours (suggests biliary excretion). Remaining ^{14}C DBDPO was detected in tissues, mainly in muscle, skin, liver and fat. Trace amounts of radioactivity were detected in urine, the spleen and brain. Excreted material in the feces was primarily unchanged DBDPO.	European Chemicals Bureau, 2002	Study details reported in a secondary source; 9.5% of the administered dose was found in the tail indicating that the dose was delivered incompletely and an unknown amount was given through the tail vein.
		Intravenous study in F344/N rats injected with 0.9 mg/kg ^{14}C DBDPO 7.17% of administered dose was detected in the bile within 4 hours. Rate of excretion was 2.2% of the dose per hour. Metabolite identification was not carried out in this study	European Chemicals Bureau, 2002	Study details reported in a secondary source; 5.38 % of the administered dose was found in the tail indicating that the dose was delivered incompletely and an unknown amount was given through the tail vein.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Sprague-Dawley rats given single oral dose of 6 µmol/kg (~2.9 mg/kg) ^{14}C DBDPO. Major route of excretion (~90% of the dose within 3 days) was via the feces, with only minor amounts (<0.05% of the dose) excreted via urine. Excretion via bile was ~9.5% of dose within 3 days. ~3% of total administered radioactivity was detected in tissues 3 days after dosing (liver (~0.9%), muscle (~0.7%), skin (~0.4%), adipose tissue (~0.3%), colon wall (~0.25%), jejunum wall (~0.05%), jejunum content (~0.05%), with minor amounts (<0.05%) in plasma, kidney, heart, lung, adrenals, testis, red blood cells, thymus and spleen). 8 phenolic metabolites were present in feces, but the majority of radioactivity was identified as unchanged DBDPO. DBDPO was metabolized via debromination	European Chemicals Bureau, 2002	Study details reported in a secondary source.
		Rats were fed diets containing 1.0 mg/kg-day technical decabromodiphenyl ether for 2 years. 3-fold higher bromine concentrations in adipose tissue, suggesting that bioaccumulation is low but retention in body fat may be pronounced.	Darnerud, 2001	Sufficient study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Inhalation	Although pulmonary exposure may occur as a result of small particle size (<5 µm), systemic absorption via this route is unknown.	European Chemicals Bureau, 2002	Brief statement reported in a secondary source.
	Other	Study conducted to study levels of PBDEs in human breast milk. Mean concentration of DecaBDE was 0.9 ng/g lw (1.2% of total PBDEs in the milk), suggesting that some decaBDE] is absorbed, distributed to mammary tissue and secreted in human breast milk during lactation.	EPA, 2008	Reported in a secondary source. Information is from monitoring data in human populations. No measured dosing studies have been conducted to determine if BDE-209 distributes to other tissues as well.
		Milk samples collected from 40-first time mothers with 8 week old infants. Mean and total concentrations of 12 tri-through decaBDE congeners were 96 and 50 ng/g lw, respectively. BDE-47 was found at the highest level, followed by hexaBDE and pentaBDE-99 and 100. DecaBDE-209 was a minor congener in breast milk (0.8 and 0.4 ng/g lw, respectively)	EPA, 2008	Reported in a secondary source. Information is from monitoring data in human populations. No measured dosing studies have been conducted to determine if BDE-209 distributes to other tissues as well.
Acute Mammalian Toxicity		**LOW: Based on acute oral and dermal LD_{50} values >2000 mg/kg in rats and rabbits and an acute inhalation LC_{50} >48.2 mg/L in rats.**		
Acute Lethality	**Oral**	Rat LD_{50} >2,000 mg/kg	European Chemicals Bureau, 2002	Reported in a secondary source; guideline study.
		Rat LD_{50} >5,000 mg/kg	European Chemicals Bureau, 2002	Reported in a secondary source; non-guideline study; necropsies were not performed.
	Dermal	Rabbit LD_{50} >2,000 mg/kg	European Chemicals Bureau, 2002	Reported in a secondary source; non-guideline study. Clinical signs of toxicity were not reported and necropsies were not performed.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Inhalation	Rat 1-hour LC_{50} >48.2 mg/L dust Spartan rats exposed for 1 hour to 2,000 or 48,200 mg/m^3 (2.0 or 48.2 mg/L) dust; No deaths or effect on body weight; Dyspnea, ocular discharge, and eye squint, increased motor activity were observed at 48.2 mg/L	European Chemicals Bureau, 2002	Reported in a secondary source; non-guideline study. Necropsy was not performed and the particle size distribution was not given.
		Single intratracheal injection to male Sprague Dawley rats (n = 50) Dose: 20 mg decabromodiphenyl ether (77.4%) dust (length mean diameter 3.17 μm). Scattered focal aggregates of alveolar macrophages in the lungs showing clear, angulated, cytoplasmic vacuoles; slight thickening of the interalveolar septae.	European Chemicals Bureau, 2002	Reported in a secondary source; non-guideline study.
Carcinogenicity		**MODERATE: Based on NTP determinations of equivocal evidence of carcinogenicity in male mice (increased incidence of hepatocelluar adenomas or carcinomas and thyroid gland follicular cell adenomas or carcinomas) and some evidence of carcinogenicity in male and female rats (increased incidences of non-neoplastic nodules in the liver). Classified as "Suggestive evidence of carcinogenic potential" by IRIS.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)			No data located.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Combined Chronic Toxicity/ Carcinogenicity	2-year carcinogenicity study (dietary) in B6C3F1 mice (50/sex/group). Doses: 0, 25,000, 50,000 ppm Average daily consumption: Males: 0, 3,200 and 6,650 mg/kg Females: 0, 3,760 and 7,780 mg/kg Increased incidence of granulomas in the liver (25,000 ppm, males); centrilobular hypertrophy with enlarged hepatocytes with frothy vacuolated cytoplasm (25,000 and 50,000 ppm, males); follicular cell hyperplasia of the thyroid gland (25,000 and 50,000 ppm, males); and increased incidence of stomach ulcers (50,000 ppm, females). No clinical signs of toxicity and no adverse effects on survival, food consumption or body weight. No evidence of carcinogenicity in females. NOAEL: not established LOAEL: 25,000 ppm based on increased incidence of non neoplastic lesions in several tissues in males	NTP, 1986; European Chemicals Bureau, 2002	Study details provided in secondary sources; guideline study in accordance with GLP procedures. NTP concludes that there was *equivocal evidence of carcinogenicity* for male mice based on increased combined incidence of both hepatocelluar adenomas and carcinomas in the low dose group and on thyroid gland follicular cells adenomas or carcinomas (combined) in both groups.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		2-year carcinogenicity study (dietary) in Fisher 344/N rats (50/sex/group) Doses: 0, 25,000, 50,000 ppm Average daily consumption: Males: 0, 1,120 and 2,240 mg/kg Females: 0, 1,200 and 2,550 mg/kg Increased incidence of thrombosis and degeneration in the liver without foci of necrosis associated and fibrosis of the spleen and lymphoid hyperplasia of the mandibular lymph nodes (50,000 ppm, males); hematopoiesis in the spleen (25,000 and 50,000 , female); acanthosis of the fore stomach (25,000 and 50,000, males); and dose dependent decreased incidence of C-cell hyperplasia of the thyroid gland (males). No clinical signs of toxicity and no compound-related effects on survival. NOAEL (systemic): 25,000 ppm LOAEL (systemic): 50,000 ppm based on neoplastic lesions, degeneration in the liver, spleen fibrosis, lymphoid hyperplasia of the mandibular lymph nodes LOAEL (local effects): 25,000 ppm based on the slight increase in fore stomach acanthosis	NTP, 1986; European Chemicals Bureau, 2002	Study details provided in secondary sources; guideline study in accordance with GLP procedures. NTP concludes that there was *some evidence of carcinogenicity* for male and female rats based on increased incidences of non-neoplastic nodules in the liver in the low dose males and high dose males and females.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Classified as "Suggestive evidence of carcinogenic potential" by EPA IRIS; weight of evidence suggests carcinogenicity and the potential for possible carcinogenic effects in humans	EPA, 2008	Summary of overall weight of evidence reviewed by IRIS.
Genotoxicity		**LOW: Based on negative results for gene mutations in bacterial and mammalian cells and lack of chromosomal aberrations in CHO cells *in vitro*.**		
	Gene Mutation *in vitro*	Negative in *Salmonella typhimurium* strains TA98, TA100, TA1535, TA1537 and *Escherichia coli* WP2 *uvrA* in the presence or absence of exogenous metabolic activation. No evidence of cytotoxicity.	European Chemicals Bureau, 2002; EPA, 2008	Guideline study in accordance with GLP procedures; study details reported in a secondary source.
		Positive in *Salmonella typhimurium* strains TA1535, TA98, TA100) in the presence or absence of exogenous metabolic activation. Doses: 50, 150, 500, 1500, 5000 µg/plate	European Chemicals Bureau, 2002	Positive results were only observed at 500 µg/plate and may be a result of the presence of an impurity. In addition, the purity decabromodiphenyl ether used in the study is unknown (data reported in a secondary source).
		Negative in *Saccharomyces cerevisiae* with and without metabolic activation	Darnerud, 2001	Study details provided in summary reported in a secondary source.
		Negative, mouse lymphoma L 5178 Y/TK+/- assay Doses: 7, 8, 9, 10 µg/plate in DMSO	European Chemicals Bureau, 2002; EPA, 2008	Guideline study in accordance with GLP procedures. Results may be weighted less heavily due to the narrow range of test concentrations used in the study; study details reported in a secondary source.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	Negative, sister chromatid exchange/chromosomal aberrations in CHO cells in the presence or absence of exogenous metabolic activation. Doses: 50, 100, 200, 500 µg/ml in DMSO	European Chemicals Bureau, 2002; EPA, 2008	Guideline study in accordance with GLP procedures; study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Chromosomal Aberrations *in vivo*	Negative, mammalian chromosomal aberration test in rat bone marrow cells. Doses: 3, 30, 100 mg/kg/day in diet	European Chemicals Bureau, 2002	Limited study details reported in a secondary source.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: Based on a LOAEL of 500 mg/kg-day in mice for adverse effects on sperm and no adverse reproductive effects following 13 week and 2 year exposures in rats and mice.**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Reproduction and Fertility Effects	One generation reproductive study in Sprague Dawley rats (10 males, 20 females in low dose groups; 15 males, 30 females in high dose groups). Doses: 0, 3, 30 or 100 mg decabromodiphenyl ether/kg body weight/day in the diet. Study duration: 60 days prior to mating, 15 days during mating, and throughout gestation and weaning. No adverse effects on fertility NOAEL: 100 mg/kg/day LOAEL: not established as highest dose tested did not produce adverse effects	European Chemicals Bureau, 2002	Reported in a secondary source. Results may be weighted less heavily due to the fact that the highest dose tested did not produce parental toxicity. In addition, individual data were not available (only a summary provided in secondary source).

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Oral gavage study in male CD-1 mice (50/group) Doses: 0, 10, 100, 500 or 1500 mg/kg-day on PNDs 21-70 Reduced amplitude of sperm lateral head displacement, reduced sperm mitochondrial membrane potential, increased sperm H2O2 generation. NOAEL: 100 mg/kg-day LOAEL: 500 mg/kg-day	EPA, 2008	Study details reported in a secondary source.
		13 week and 2 year carcinogenicity studies in B6C3F1 mice and F344/N rats did not produce adverse macroscopic or histological changes in the testes, prostate ovaries, or uterus. Doses: 0, 3,100, 6,200, 12,500, 25,000, 50,000 ppm (13 week study) or 0, 25,000 or 50,000 ppm (2 year studies)	NTP, 1986; European Chemicals Bureau, 2002	Guideline studies reported in a secondary source.
Developmental Effects		**HIGH: A number of rodent developmental neurotoxicity studies addressing decaBDE exposure have been published and are listed below. The hazard designation for this endpoint was assigned based upon the most conservative NOAEL and LOAEL values in the located studies. The adverse effects in these studies were reduced thyroid hormone levels and abnormal behavior activity. This aligns with the assessment for decaBDE published by EPA's Integrated Risk Information System (IRIS).**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Prenatal Exposure	Oral gavage study in pregnant Sprague Dawley rats (n = 20) Dose: 0, 10, 100 or 1,000 mg decabromodiphenyl ether/kg body weight/day Study duration: GD 6-15 Statistically significant increase in resorptions (10 mg/kg/day) No gross external abnormalities. Significant increase in the numbers of litters with subcutaneous edema and delayed ossification of normally developed bones of the skull (1,000 mg/kg/day) NOAEL (maternal) = 1,000 mg/kg/day LOAEL (conceptus) = 10 mg/kg/d	European Chemicals Bureau, 2002	Study results may be weighted less heavily due to the low compound purity; test substance identified as a commercial mixture (77.4% decabromodiphenyl ether, 21.8% nonabromodiphenyl ether, 0.8% octabromodiphenyl ether) used in the study), which is lower than the purity of the products currently supplied in the EU. Study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Oral gavage study in pregnant Sprague Dawley rats (25/group) Dose: 0, 100, 300 or 1,000 mg/kg/day of decabromodiphenyl ether (purity of 97.34%) Study duration: GD 0-19 No adverse maternal clinical findings or effects on body weight, body weight gain or liver weights. No adverse treatment-related effects on external malformations or variations, skeletal variation or ossification. No adverse effects on fetal weight, sex ratio, total/late resorptions. NOAEL (maternal, developmental): 1,000 mg/kg-day	European Chemicals Bureau, 2002; EPA, 2008	Guideline study in accordance with GLP procedures. Study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Oral gavage (corn oil) study in rats, 0, 100, 300, 1,000 mg/kg/day, (half exposed GD6-20, other half exposed GD6- through LD 4). No maternal treatment-related effects on mortality, clinical signs of toxicity, body weight, body weight gain, or food consumption. No effects on gestational or litter parameters (mean gestational length, mean number of pups born, percentage of males at birth, mean live litter size, postnatal survival, mean offspring body weight and weight gains through PND 21). NOAEL = 1,000 mg/kg/day (highest dose tested)	Biesemeier et al. 2010	LOAEL not identified.
		Rat, neurodevelopmental study, oral (gavage) administered 0, 1, 10, 100, or 1,000 mg/kg/day, GD 6 through weaning. No treatment-related neurobehavioral effects were observed (startle response, learning, and memory tests assessed); No changes in were reported in motor activity evaluations at 2,4, or 6 months of age; No neuropathological or morphometric changes reported. NOAEL = 1,000 mg/kg/day (highest dose tested)	Biesemeier et al. 2011	LOAEL not identified.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Postnatal Exposure	Evaluation of locomotor activity in C57BL6/J mice Dose: 0, 6 or 20 mg/kg on PNDs 2-15 with observation after placement in a novel environment on PND70 No adverse effects on developmental endpoints (on pinnae detachment, incisor eruption, eye opening, vaginal opening or testes descent). Declined locomotor activity in males and females on PND70 (decline was significantly different for males at 6 and 20 mg/kg compared to controls); Decreased % of pups performing the palpebral reflex on PND 14, increased struggling behavior (males) on PND20, decreased T4 levels (males) on PND70. NOAEL: not established LOAEL: 6 mg/kg-day (based on decreased T4 levels in male mice and effects on locomotor activity in male mice on PND 70	EPA, 2008; Washington DOE, 2008	Study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Single dose gavage in male Sprague Dawley rats (20 rats from 3-5 litters/group) Doses: 0, 6.7 or 20.1 mg/kg on PND3 Dose-related disruption in habituation (changes in locomotion, rearing, total activity) at both doses. NOAEL: Not established LOAEL: 6.7 mg/kg	EPA, 2008	Each dose administered a single time; not a guideline study. Study details reported in a secondary source.
		NMRI male mice (10 mice from 3-5 litters/group) gavaged with decabromodiphenyl ether (99% pure) at 0, 2.22, or 20.1 mg/kg on PNDs3-19 or 0, 1.34, 13.4 or 20.1 mg/kg on PND10. Dose-related disruption in habituation (changes in locomotion, rearing, total activity) at 2, 4, and 6 months following exposure to 20.1 mg/kg on PND3. NOAEL (NMRI mice): 2.22 mg/kg LOAEL (NMRI mice: 20.1 mg/kg	EPA, 2008	Each dose administered a single time; not a guideline study. Study details reported in a secondary source.
Neurotoxicity		**HIGH: A number of rodent developmental neurotoxicity studies addressing decaBDE exposure have been published and are listed below. The hazard designation for this endpoint was assigned based upon the most conservative NOAEL and LOAEL values in the located studies. The adverse effects in these studies were reduced thyroid hormone levels and abnormal behavior activity. This aligns with the assessment for decaBDE published by EPA's Integrated Risk Information System (IRIS).**		
	Neurotoxicity Screening Battery (Adult)			No data located.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Developmental Neurotoxicity	Evaluation of locomotor activity in C57BL6/J mice Dose: 0, 6 or 20 mg/kg BDE-209 on PNDs 2-15 with observation after placement in a novel environment on PND70 and using special functional observational battery (FOB) No effects on pinnae detachment, incisor eruption, eye opening, vaginal opening, or testes descent. Increased locomotor activity in males and decreased activity in females (PND 70) when exposed to 6 and 20 mg/kg-day. Locomotor activity of 1-year old mice (male and female) did not differ from controls. Decreased % of pups (male and female) adequately performed the palpebral reflex (PND 14) compared to controls (6 or 20 mg/kg-day). Decreased number of pups (males) adequately performed an effective forelimb grip (PND 14 and 16) compared with same-sex controls (20 mg/kg-day). Increased struggling behavior (males and females) on PND20 (6 mg/kg-day). Decreased T_4 levels (males) on PND70. NOAEL: not established LOAEL: 6 mg/kg-day	EPA, 2008; Washington DOE, 2008	Study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Single dose gavage in male Sprague Dawley rats (20 rats from 3-5 litters/group) Doses: 0, 6.7 or 20.1 mg/kg on PND3 Dose-related disruption in habituation (changes in locomotion, rearing, total activity) at both doses at 2,4, and 6 months of age. NOAEL: not established LOAEL: 6.7 mg/kg	EPA, 2008	Each dose administered a single time; not a guideline study. Study details reported in a secondary source.
		Rat, neurodevelopmental study, oral (gavage) administered 0, 1, 10, 100, or 1,000 mg/kg/day, GD 6 through weaning; No treatment-related neurobehavioral effects were observed (startle response, learning, and memory tests assessed); No changes in were reported in motor activity evaluations at 2,4, or 6 months of age; No neuropathological or morphometric changes reported. NOAEL = 1,000 mg/kg/day (highest dose tested)	Biesemeier et al. 2011	A LOAEL was not identified.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		NMRI male mice (10 mice from 3-5 litters/group) gavaged with decabromodiphenyl ether (99% pure) at 0, 2.22, or 20.1 mg/kg on PNDs 3 and 19 or 0, 1.34, 13.4 or 20.1 mg/kg on PND 10 Dose-related disruption in habituation (changes in locomotion, rearing, total activity) at 2, 4, and 6 months following exposure to 20.1 mg/kg on PND3. NOAEL (NMRI mice): 2.22 mg/kg LOAEL (NMRI mice: 20.1 mg/kg	European Chemicals Bureau, 2002; EPA, 2008	Each dose administered a single time; not guideline study. Study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects	**MODERATE: Based on a LOAEL of 80 mg/kg-day for adverse liver and thyroid effects following a 30-day oral exposure in rats. A NOAEL was not established in the 2-year carcinogenicity study. The LOAEL of 3,200 mg/kg/day yields uncertainty to the dose levels where adverse effects may begin. These subchronic effects appear consistent with the observed chronic effects although the latter was observed at higher doses.**		
	30-day dietary study in male Sprague-Dawley rats (number/group not specified) Doses: 0, 100, 1,000, 10,000 ppm (~0, 8, 80, 800 mg/kg/day) Enlarged livers (1,000 ppm); thyroid hyperplasia (1,000 and 10,000 ppm); hepatic centrilobular cytoplasmic enlargement and vacuolisation and renal hyaline degenerative cytoplasmic changes (10,000 ppm). No clinical signs of toxicity and no adverse effects on food consumption, body weight, organ weight or hematological/urinary parameters. NOAEL: 100 ppm (8 mg/kg/day) LOAEL: 1,000 ppm (80 mg/kg/day) based on incidence of enlarged livers	European Chemicals Bureau, 2002; EPA, 2008	Results may be weighted less heavily due to the low compound purity (77.4% decabromodiphenyl ether - 21.8% nonabromodiphenyl oxide) used in the study, which is lower than the purity of the products currently supplied in the EU; study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	14-day dietary study in B6C3F1 mice and F344/N rats (5/sex/group). Doses: 0, 5,000, 10,000, 20,000, 50,000, or 100,000 ppm decabromodiphenyl ether (99% purity). Estimated average doses: **Mice:** 0, 1,027, 2,143, 4,246, 10,536, or 20,994 mg/kg-day in male mice and 0, 1,146, 2,286, 4,627, 11,348, or 23,077 mg/kg-day in female mice. **Rats:** 0, 472, 928, 1,846, 4,569, or 9,326 mg/kg-day in male rats and 0, 538, 1,061, 2,137, 5,323, or 10,853 mg/kg-day in female rats. No adverse effects on health, survival body weight, clinical signs or gross pathology. NOAEL (mice): 20,994 mg/kg-day in male mice and 23,077 mg/kg-day in female mice LOAEL: Not established, as highest dose tested did not produce adverse effects NOAEL(rats): 9,326 mg/kg-day in male rats and 10,853 mg/kg-day in female rats LOAEL: Not established, as highest dose tested did not produce adverse effects	European Chemicals Bureau, 2002; Maine, unpublished; EPA, 2008	Guideline study in accordance with GLP procedures; study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	13-week dietary study in B6C3F1 mice and F344/N rats (10/sex/group) Doses: 0, 3,100, 6,200, 12,500, 25,000, 50,000 ppm Estimated average doses: **Mice:** 0, 666, 1,355, 2,659, 5,278, or 10,233 mg/kg-day in males and 0, 702, 1,437, 2,899, 5,687, or 11,566 mg/kg-day in females **Rats:** 0, 191, 372, 781, 1,536, or 3,066 mg/kg-day in male rats and 0, 238, 504, 967, 1,955, or 3,944 mg/kg-day in female rats No adverse effects on health, survival body weight, clinical signs or gross pathology. NOAEL (mice): 10,233 mg/kg-day in males and 11,566 mg/kg-day in females LOAEL (mice): Not established, as highest dose tested did not produce adverse effects NOAEL (rats): 3,066 mg/kg-day in male rats and 3,944 mg/kg-day in female rats LOAEL (rats): Not established, as highest dose tested did not produce adverse effects	European Chemicals Bureau, 2002; Maine, unpublished; EPA, 2008	Guideline study in accordance with GLP procedures; study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	28-day dietary study in F344/N rats (10/sex/group) Doses: 0, 100, 1,000 ppm (0, 7, 70 mg/kg/day (M); 0, 8, 80 mg/kg/day (F)) No adverse effects on health, survival body weight, food consumption, behavior, or gross pathology. NOAEL: 1,000 ppm (70 or 80 mg/kg-day for males and females, respectively) LOAEL: Not established, as highest dose tested did not produce adverse effects	European Chemicals Bureau, 2002; EPA, 2008	Guideline study; study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	2-year carcinogenicity study (dietary) in B6C3F1 mice (50/sex/group) Doses: 0, 25,000, 50,000 ppm Average daily consumption: Males: 0, 3,200 and 6,650 mg/kg/day Females: 0, 3,760 and 7,780 mg/kg/day Increased incidence of granulomas in the liver (25,000 ppm, males); centrilobular hypertrophy with enlarged hepatocytes with frothy vacuolated cytoplasm (25,000 and 50,000 ppm, males); follicular cell hyperplasia of the thyroid gland (25,000 and 50,000 ppm, males); increased incidence of stomach ulcers (50,000 ppm, females) No clinical signs of toxicity and no adverse effects on survival, food consumption or body weight. NOAEL: Not established LOAEL: 25,000 ppm (3,200 mg/kg-day) based on increased incidence of non neoplastic lesions in several tissues	European Chemicals Bureau, 2002; EPA, 2008	Guideline study in accordance with GLP procedures; study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	2-year carcinogenicity study (dietary) in Fisher 344/N rats (50/sex/group) Doses: 0, 25,000, 50,000 ppm Average daily consumption: Males: 0, 1,120 and 2,240 mg/kg Females: 0, 1,200 and 2,550 mg/kg Increased incidence of thrombosis and degeneration in the liver without foci of necrosis associated, fibrosis of the spleen and lymphoid hyperplasia of the mandibular lymph nodes (50,000 ppm, males); hematopoiesis in the spleen (25,000 and 50,000 , female); acanthosis of the fore stomach (25,000 and 50,000, males); dose dependent decreased incidence of C-cell hyperplasia of the thyroid gland (males). No clinical signs of toxicity and no compound-related effects on survival NOAEL (systemic): 25,000 ppm (1,120 mg/kg-day) LOAEL (systemic): 50,000 ppm (2,240 mg/kg-day) based on neoplastic lesions, degeneration in the liver, spleen fibrosis, lymphoid hyperplasia of the mandibular lymph nodes LOAEL (local effects): 25,000 ppm (1,120 mg/kg-day) based on the slight increase in fore stomach acanthosis	European Chemicals Bureau, 2002; EPA, 2008	Guideline study in accordance with GLP procedures; study details reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		4-day oral gavage study in Long-Evans female weanling rats (8/group). Doses: 0, 0.3, 1, 3, 10, 30, 60 or 100 mg/kg-day No dose-related effects on body weight, liver weight or changes in T3 or T4 levels. NOAEL: 100 mg/kg/day LOAEL: not established, as highest dose tested did not produce adverse effects	EPA, 2008	A 4-day exposure study may not a good indicator of chronic exposure effects; study details reported in a secondary source.
Skin Sensitization		**LOW: Based on negative results for skin sensitization in guinea pigs and human volunteers.**		
	Skin Sensitization	Negative, guinea pigs	European Chemicals Bureau, 2002	Reported in a secondary source; study was performed using a mixture of polybrominated diphenyl oxides (commercial octaBDE) which comprised of <3% decabromodiphenyl ether.
		Negative, human volunteers	European Chemicals Bureau, 2002	Reported in a secondary source; concentrations tested were very low (2-5%).
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Decabromodiphenyl ether is a mild eye irritant in rabbits.**		
	Eye Irritation	Transient, mild irritation, rabbits (reversible in 48 hours)	European Chemicals Bureau, 2002	Reported in a secondary source; guideline study in accordance with GLP procedures.
Dermal Irritation		**LOW: Decabromodiphenyl ether is a slight skin irritant in humans.**		
	Dermal Irritation	Non-irritant, rabbit	European Chemicals Bureau, 2002	Reported in a secondary source; guideline study using commercial decabromodiphenyl ether as dry solid.
		Slight irritation, human volunteers	European Chemicals Bureau, 2002	Reported in a secondary source.

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PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Endocrine Activity	**Limited studies were located on the ability of decabromodiphenyl ether to interact with the endocrine system. However, some metabolites of decabromodiphenyl ether are known to produce estrogenic effects. In addition, decabromodiphenyl ether is listed as a potential endocrine disrupter on the EU Priority List of Suspected Endocrine Disrupters and on the Red List of chemicals.**		
	Pimephales promelas (fathead minnows) fed 0.16 µg/g BDE-209 for 28 days. Reduced rates of outer and inner ring deiodination of thyroxine (74%). Significantly increased thyroid follicular epithelial cell heights	Noyes et al., 2011	Study details from primary source.
	Ongoing unpublished studies at the University of Southern Maine indicate effects on blood concentrations of hormone T_4 in male mice and no effects on treated females.	Maine, unpublished	This is an ongoing study at the University of Southern Maine. No definitive conclusions regarding the potential for decabromodiphenyl ether to produce endocrine disruption have been made.
	Decabromodiphenyl ether is listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.	European Commission, 2012	"Potential for endocrine disruption. In vitro data indicating potential for endocrine disruption in intact organisms. Also included effects in-vivo that may, or may not, be endocrine disruption-mediated. May include structural analyses and metabolic considerations".

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Immunotoxicity		**Histological changes in lymphoid organs occurred at 2,240 mg/kg-day in a chronic study of rats.**		
	Immune System Effects	In chronic dietary studies in male rats, decabromodiphenyl ether has caused histological changes in lymphoid organs (spleen, mandibular lymph nodes) at 2,240 mg/kg-day.	EPA, 2008	Study details reported in a secondary source.
		No cytotoxic effects in splenocytes from C57BL/6 mice incubated in culture with 3 µmol/L decabromodiphenyl ether (purity not specified). No attenuation of interleukin-2-receptor α chain (CD25) expression (demonstrating a lack of effect on the immune system in an immunosuppressive manner).	EPA, 2008	Study details reported in a secondary source.
ECOTOXICITY				
Aquatic Toxicity				
ECOSAR Class				
Acute Toxicity		**LOW: The log K_{ow} of the compound (6.27) exceeds the ECOSAR cutoff value of 5.0 for acute endpoints and therefore, no effects at saturation (NES) are predicted. Although experimental studies were located for fish and green algae, they were considered to be inadequate due to deviations from standard protocols and resulting toxicity values that exceed the compound's water solubility.**		
Fish LC_{50}		*Oryzias latipes* 48 hour LC_{50} >500 mg/L	European Chemicals Bureau, 2002	OECD guidelines for acute aquatic toxicity (203) state that the preferred exposure duration is 96 hours.
		96 hour LC_{50} = 0.129 mg/L (ECOSAR: neutral organics) (Estimated)	EPI	The log K_{ow} exceeds the ECOSAR cutoff value of 5.0 for acute endpoints and therefore, no effects at saturation are predicted.

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PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Daphnid LC_{50}	48 hour LC_{50} = 0.137 mg/L (ECOSAR: neutral organics) (Estimated)	EPI	The log K_{ow} exceeds the ECOSAR cutoff value of 5.0 for acute endpoints and therefore, no effects at saturation are predicted.
Other Freshwater Invertebrate LC_{50}	Mysid shrimp 96 hour LC_{50} = 0.006 mg/L (ECOSAR: neutral organics) (Estimated)	EPI	The log K_{ow} exceeds the ECOSAR cutoff value of 5.0 for acute endpoints and therefore, no effects at saturation are predicted.
Green Algae EC_{50}	*Skeletonema costatum, Thalassiosira pseudonana* 72 hour EC_{50} >1 mg/L	European Chemicals Bureau, 2002	Reported in a secondary source; the reported toxicity limit exceeds the compound's water solubility.
	Chlorella sp. 96 hour EC_{50} >1 mg/L	European Chemicals Bureau, 2002	Reported in a secondary source, the reported toxicity limit exceeds the compound's water solubility.
	96 hour EC_{50} = 0.416 mg/L (ECOSAR: neutral organics) (Estimated)	EPI	The log K_{ow} exceeds the ECOSAR cutoff value of 5.0 for acute endpoints and thus, no effects at saturation are predicted.
Chronic Aquatic Toxicity	**LOW: Based on estimated values for fish, daphnia and algae that exceed the water solubility and are therefore predicted to have no effects at saturation.**		
Fish ChV	30-day ChV = 0.018 mg/L (ECOSAR: neutral organics) (Estimated)	EPI	The ChV value exceeds the water solubility by more than a factor of 10, and therefore, no effects at saturation are predicted.
Daphnid ChV	ChV = 0.031 mg/L (ECOSAR: neutral organics) (Estimated)	EPI	The ChV value exceeds the water solubility by more than a factor of 10 and therefore, no effects at saturation are predicted.
Saltwater Invertebrate ChV	Mysid shrimp ChV = 0.00015 mg/L (ECOSAR: neutral organics) (Estimated)	EPI	This chemical may not be soluble enough to measure this predicted effect.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Green Algae ChV		ChV = 0.324 mg/L (ECOSAR: neutral organics) (Estimated)	EPI	The ChV value exceeds the water solubility by more than a factor of 10, and therefore, no effects at saturation are predicted.
Sediment Dwelling Organisms ChV		*Lumbriculus variegatus* NOEC ≥5,000 mg/kg dry weight based on nominal concentrations	European Chemicals Bureau, 2002	Reported in a secondary source; guideline study (ASTM 1706-95b and OPPTS No. 850.1736). EPA-DfE has not established hazard criteria for studies based on sediment concentrations nor sediment dwelling organisms at the time of this report.
Terrestrial Ecotoxicity				
Chicken embryo toxicity		Chicken embryo LD_{50} = 740 ng/g ww	Sifleet 2009	Test substance identified a BDE-209.
Earthworm Subchronic Toxicity		56-day NOEC (survival or reproduction) >4,910 mg/kg dry weight using nominal concentrations	European Chemicals Bureau, 2002	Reported in a secondary source; guideline study (OECD 207 test guideline).
ENVIRONMENTAL FATE				
Transport		**The transport evaluation for decabromodiphenyl ether is based on both estimated and experimental physical and chemical properties. Based on the Level III fugacity models incorporating the located experimental property data, decabromodiphenyl ether is expected to partition primarily to soil. It is not expected to dissociate at environmentally-relevant pHs. Decabromodiphenyl ether is expected to have low mobility in soil based on its estimated K_{oc}. Therefore, leaching of decabromodiphenyl ether through soil to groundwater is not expected to be an important transport mechanism. Estimated volatilization half-lives for a model river indicate that it will have moderate potential to volatilize from surface water. Volatilization potential from a model lake is expected to be low. In the atmosphere, decabromodiphenyl ether is expected to exist in both the vapor and particulate phase. Vapor-phase decabromodiphenyl ether is expected to have limited potential for photodegradation. Particulate phase decabromodiphenyl ether will be removed from air by wet or dry deposition.**		
	Henry's Law Constant (atm-m^3/mole)	4.4×10^{-4} at 25ºC (Estimated)	EPI	Value was obtained from the measured vapor pressure and water solubility.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	$2.8x10^5$ (Estimated)	EPI	
	Level III Fugacity Model	Air = <1% (Estimated) Water = 1.5% Soil = 63% Sediment = 35%	EPI	In addition to EPI estimates, these results were obtained by using the measured vapor pressure, log K_{ow}, and water solubility.
Persistence		**VERY HIGH: The persistence concern for decabromodiphenyl ether is very high; it is not expected to degrade rapidly under aerobic conditions. Slow degradation through debromination may occur under anaerobic conditions. The anaerobic experimental results are indicative of limited removal but at very low rates that are possibly background level degradation under the test conditions. Experimental studies indicate no degradation after 2 weeks in a ready biodegradation test, but no data were located for soil or water. Results from biodegradation estimation models also suggest decabromodiphenyl ether is recalcitrant under aerobic conditions. Non-guideline experimental studies indicate decabromodiphenyl ether is capable of undergoing anaerobic biodegradation; however the removal rate also suggests very high persistence. The initially formed degradation products are also expected to be persistent. Decabromodiphenyl ether is not expected to hydrolyze in the environment based on experimental data. Experimental data indicate that decabromodiphenyl ether undergoes debromination via photolysis and metabolism to lower brominated diphenyl oxides. Data concerning the kinetics of these reactions were not readily located.**		
Water	**Aerobic Biodegradation**	No degradation after 2 weeks (Measured) OECD Test Guideline 301C	MITI, 1998	Guideline study; reported 80% retention in water (control) and sludge. Study hypothesized that loss of compound is due to decabromodiphenyl ether converting to an intermediate product under the study conditions.
	Volatilization Half-life for Model River	7.3 hours (Estimated)	EPI	Estimation model was calculated using all applicable measured input values and the Henry's Law Constant obtained from the measured vapor pressure and water solubility.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Volatilization Half-life for Model Lake	340 days (Estimated)	EPI	Estimation model was calculated using all applicable measured input values and the Henry's Law Constant obtained from the measured vapor pressure and water solubility.
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation	No degradation after 4 months in incubated, acclimated anaerobic sediments (Measured)	European Chemicals Bureau, 2002	Reported in a secondary source with limited study details.
		<1% degradation after 32 weeks in anaerobic river sediments (Measured)	European Chemicals Bureau, 2002	Reported in a secondary source. Study used C-14 labeled test substance, analyzed by HPLC.
		Decabromodiphenyl ether in sewage sludge was broken down into octa and nonaBDE; study run with and without organic chemical primers; half-life ~700 days with primers, longer without primers. (Measured)	Illinois EPA, 2007 citing Gerecke et al., 2006.	Reported in a secondary source with limited study details.
		Breakdown to hexa- and nona-BDEs in anaerobic sediment cultures after 3.5 years. Half-life = 10 years. (Measured)	Illinois EPA, 2007 citing Nies et al. 2005	Reported in a secondary source with limited study details.
		Rapid breakdown to nonaBDEs in anaerobic sediment cultures in the presence of organic solvents. (Measured)	Illinois EPA, 2007 citing Skoczynska et al., 2005	Reported in a secondary source with limited study details.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Debromination of decabromodiphenyl ether was found to occur in species specific studies with *Sulfurospillum multivorans* to hepta- and octaBDEs in the presence of trichloroethylene. *Dehalococcoides* species were not able to debrominate decabromodiphenyl ether. (Measured)	Illinois EPA, 2007 citing He et al., 2006	Reported in a secondary source with limited study details.
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	320 days (Estimated)	EPI	
Reactivity	**Photolysis**	Degradation to lower brominated diphenyl ether congeners and sometimes polybrominated dibenzofurans reported under varying conditions in several laboratory studies using UV and natural sunlight. (Measured)	European Chemicals Bureau, 2002	Based on a summary of several laboratory studies under varying conditions, using UV and natural light.
		DecaBDE absorbed into clays and organic rich sediments experienced debromination in UV and natural light. Debromination of decabromodiphenyl ether absorbed on three metal oxides did not occur. (Measured)	Illinois EPA, 2007 citing Ahn et al., 2006	Reported in a secondary source with limited study details.
		No evidence of light-mediated debromination of decabromodiphenyl ether applied to soil in sewage sludge. (Measured)	Illinois EPA, 2007 citing Sellstrom et al., 2005	Reported in a secondary source with limited study details.
	Hydrolysis	No degradation at pH 5 and 7 at 100ºC after six weeks. (Measured)	European Chemicals Bureau, 2002	Reported in a secondary source.

Decabromodiphenyl Ether CASRN 1163-19-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Environmental Half-life		360 days (Estimated)	PBT Profiler, Professional judgment	Half-life estimated for the predominant compartment, as determined by EPI and the PBT Profiler methodology.
Bioaccumulation		**HIGH: Based on estimated BAF values suggesting that the potential for bioaccumulation is high and located monitoring data indicating that decabromodiphenyl ether has been detected in higher trophic level organisms. Experimental studies indicate limited uptake from food. Decabromodiphenyl ether degradation, transformation and metabolism products also contribute to the high bioaccumulation hazard designation. These compounds are lower brominated congeners and also have been detected in monitoring studies (ATSDR, 2004).**		
	Fish BCF	<5 to <50 (Measured) Using MITI Test; 6 week exposure in *Cyprinus carpio* with Decabromodiphenyl ether concentrations of 60 ppb and 6 ppb, respectively	MITI, 1998	Guideline study that may have been performed above the water solubility of the test substance.
	BAF	49,000 (Estimated)	EPI	
	Metabolism in Fish	Little or no uptake from water phase exposure; limited uptake (~0.02-0.13%) observed when exposed from food, after 120-day exposure period. (Measured)	European Chemicals Bureau, 2002	Reported in a secondary source.
		Found to be metabolized in juvenile fathead minnows and to accumulate after 28-day treatment at 9.8 µg/g food. A range of penta- to octaBDEs metabolites were detected with 2,2',4,4',5,6'-hexabromodiphenyl ether being most prevalent (Measured)	Noyes et. al., 2011	Adequate, non guideline study.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		Detected in surface water particulates; wet and dry deposition samples; sludge and effluents from wastewater treatment plants; sediments and soils worldwide; urban, rural, and suburban atmospheric air; indoor air (HSDB, 2011).		

Decabromodiphenyl Ether CASRN 1163-19-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Ecological Biomonitoring	Detected in tree bark; fish and shellfish worldwide; in cats; owl and peregrine falcon eggs in Belgium and Sweden , respectively (HSDB, 2011); peregrine falcon eggs in California (Park et al., 2009); birds of prey, herbivore and predator mammals, marine fish, marine invertebrates, marine mammals, marine/aquatic/other birds and vegetation (Canada, 2010).		
Human Biomonitoring	Detected in breast milk (HSDB, 2011). This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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Ethylene Bis-Tetrabromophthalimide (EBTBP)

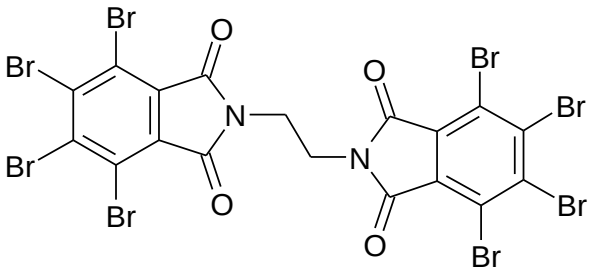
Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.
§ Based on analogy to experimental data for a structurally similar compound.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Ethylene Bis-Tetrabromophthalimide	32588-76-4	L	*M*§	L	*L*	L	*M*§	L	*L*		VL	VL	*L*	*L*	VH	*H*

Ethylene Bis-Tetrabromophthalimide (EBTBP)



CASRN: 32588-76-4

MW: 951.5

MF: $C_{18}H_4Br_8N_2O_4$

Physical Forms: Solid
Neat:

Use: Flame retardant

SMILES: O=C1N(C(=O)c2c(c(c(c(c12)Br)Br)Br)Br)CCN1C(=O)c2c(c(c(c(c2Br)Br)Br)Br)C1=O

Synonyms: 1H-Isoindole-1,3(2H)-dione, 2,2'-(1,2-ethanediyl)bis[4,5,6,7-tetrabromo- (TSCA Inventory); Saytex BT 93; Ethylene bis(tetrabromophthalimide); 2,2'-(1,2-Ethanediyl)bis(4,5,6,7-tetrabromo-1H-isoindole-1,3(2H)-dione); N,N'-Ethylenebis(3,4,5,6-tetrabromophthalimide)

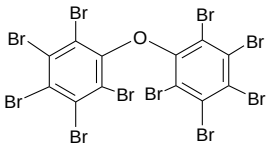
Chemical Considerations: This alternative is a discrete organic chemical with a MW below 1000. EPI v 4.1 was used to estimate physical-chemical and fate values. No measured values were incorporated due to an absence of experimental data.

Polymeric: No
Oligomers: Not applicable

Metabolites, Degradates and Transformation Products: None

Analog: Decabromodiphenyl ether (1163-19-5) and other confidential analogs
Endpoint(s) using analog values: Neurotoxicity; Carcinogenicity

Analog Structure:



Decabromodiphenyl ether
1163-19-5

Additional analogs are confidential and cannot be suitably represented here.

Structural Alerts: None identified

Risk Phrases: Not classified by Annex I Directive 67/548/EEC & IUCLID (Pakalin, 2007)

Hazard and Risk Assessments: Risk assessment completed for Ethylene bis-tetrabromophthalimide (EBTBP) by Denmark in 2007 (Stuer-Lauridsen, 2007) and a dossier was completed by Albemarle Corporation for EPA's High Production Program (HPV, 2008).

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	446 (Measured)	NIEHS, 1999	Non guideline study, yet established method considered sufficient for a screening assessment.
Boiling Point (°C)	>300 (Estimated)	EPI; EPA, 1999	Cutoff value for high boiling point compounds according to HPV assessment guidance.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	EPI; EPA, 2011	Cutoff value for non volatile compounds according to SF assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	EPI; EPA, 1999	Cutoff value for non soluble compounds according to HPV assessment guidance.
Log K_{ow}	9.8 (Estimated)	EPI; EPA, 2011	Near cutoff value for non soluble compounds according to SF assessment guidance.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_b	5.48 (Estimated)	SPARC	
HUMAN HEALTH EFFECTS			
Toxicokinetics	**Ethylene bis-tetrabromophthalimide as a neat material is estimated to not be absorbed by any route of exposure and is expected to have poor absorption for all routes when in solution. Ethylene bis-tetrabromophthalimide is distributed through tissues, but dissipates after exposure ceases; it is excreted primarily in the feces and urine. There were no data located regarding absorption or metabolism.**		
Dermal Absorption *in vitro*			No data located.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No absorption through all routes as neat material; poor absorption through all routes when in solution	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/chemical properties.
		Rat, oral (gavage), 14-day exposure to 14C-labelled BT93; excreted primarily in the feces (65% of total dose) and urine (15% of total dose); minor amounts of 14C-label was found in tissues, but dissipated within the 30-day withdrawal period.	NIEHS 1999; IUCLID 2000	Reported in a secondary source with limited study details.
Acute Mammalian Toxicity		**LOW: Based on acute oral and dermal LD_{50} values of >2000 mg/kg and the inhalation LC_{50} value of >20 mg/L.**		
Acute Lethality	**Oral**	Rat oral LD_{50} >5,000 mg/kg	IUCLID 2000	Reported in a secondary source; limited study details provided.
		Rat oral LD_{50} >7,500 mg/kg	NIEHS 1999; HPV 2008	Reported in a secondary source; some study details provided.
	Dermal	Rabbit dermal LD_{50} >2,000 mg/kg	IUCLID 2000	Reported in a secondary source; some study details provided.
	Inhalation	Rat inhalation 1 hr LC_{50} >203 mg/L	NIEHS 1999; IUCLID 2000	Reported in a secondary source; limited study details provided; not the preferred 4-hour exposure.
Other Acute Effects		Rat 1-hour inhalation to a dust atmosphere of ehtylenebis (tetrabromophthalimide) of 4,500 ± 3,000 mg/m^3 resulted in dyspnea, and dry, red, brown matter around the muzzle. There were no changes in body weight gain during a 14-day observation period. LOAEL = 4,500± 3,000 mg/m^3	NIEHS 1999	Reported in a secondary source; limited study details provided; the rats were only exposed to one concentration of the test substance and the mean concentration the rats were exposed to was quite variable, as indicated by a large standard deviation.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Carcinogenicity		**MODERATE: Estimated to have a marginal potential for carcinogenicity based on professional judgment. There is potential for carcinogenicity estimated based on the high potential for bioaccumulation and potential for expression of adverse effects in longer term studies. No experimental carcinogenicity data regarding exposure to ethylene bis-tetrabromophthalimide were located.**		
	OncoLogic Results			Not amenable to available estimation method.
	Carcinogenicity (Rat and Mouse)	Marginal potential for oncogenicity. (Estimated by analogy)	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/chemical properties.
		Potential for carcinogenicity; increased incidence of neoplastic nodules of the liver in rats; equivocal evidence of increased incidences of hepatocellular adenomas or carcinomas and thyroid gland follicular cell adenomas or carcinomas in male mice. (Estimated by analogy)	Professional judgment	Estimated based on the high potential for bioaccumulation and by analogy to observations on decabromodiphenyl ether where adverse effects were not present in 90-day studies but were expressed following chronic exposure in a NTP study.
	Combined Chronic Toxicity/ Carcinogenicity			No data located.
Genotoxicity		**LOW: Ethylene bis-tetrabromophthalimide did not cause mutations in bacterial cells or chromosomal aberrations in mammalian cells *in vitro*.**		
	Gene Mutation *in vitro*	Negative, *S. typhimurium* TA98, TA100, TA1535, TA1537, TA1538; *E. coli* WP2uvrA with and without metabolic activation.	NIEHS 1999; IUCLID 2000; HPV 2008; CCRIS 2011; NTP 2011	Reported in secondary sources; sufficient study details provided.
		Negative, *S. typhimurium* TA98, TA1535, TA1537 with and without metabolic activation.	Zeiger et al. 1985	Reported in a primary source; adequate study details provided.
		Negative, *S. typhimurium* TA98, TA100, TA1535, TA1537, TA1538; *S. cerevisiae* D4 with and without metabolic activation.	NIEHS 1999; IUCLID 2000; HPV 2008	Reported in a secondary source; sufficient study details provided.
	Gene Mutation *in vivo*			No data located.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Chromosomal Aberrations *in vitro*	Negative, Chinese hamster ovary (CHO) cells with and without metabolic activation.	HPV 2008	Reported in a secondary source; sufficient study details provided.
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: Based on professional judgment, there is no potential for reproductive toxicity.**		
	Reproduction/ Developmental Toxicity Screen	Low potential for reproductive toxicity. (Estimated)	Expert judgment	Estimated based on expert judgment.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			
Developmental Effects		**LOW: Ethylene bis-tetrabromophthalimide did not cause developmental effects in rats or rabbits following gestational exposure at oral doses as high as 1,000 mg/kg bw-day. Based on professional judgment, there is no potential for developmental toxicity.**		
	Reproduction/ Developmental Toxicity Screen	There is no evidence of developmental toxicity (Estimated by analogy)	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/chemical properties.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Prenatal Development	Sprague-Dawley rats (25/group) were administered ethylene bis-tetrabromophthalimide by gavage at 0, 100, 500, 1,000 mg/kg bw-day on GD 6-15. There were no treatment-related effects on maternal survival, body weight gains, food consumption. There were no treatment-related changes in intrauterine survival and fetal weight, and no changes in the incidence of developmental malformations and variations compared to controls Parental toxicity: NOAEL >1,000 mg/kg bw-day (highest dose tested) Reproductive toxicity: NOAEL >1,000 mg/kg bw-day (highest dose tested)	NIEHS 1999; IUCLID 2000; HPV 2008	Reported in secondary sources; sufficient study details provided; follows OECD guidelines. The study is in accordance with EPA OPPTS method 870.3700.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		New Zealand white rabbits (20/group) were administered ethylene bis-tetrabromophthalimide by gavage at 0, or 1,000 mg/kg bw-day on GD 7-19. There were no treatment-related effects on maternal survival, body weight gains, food consumption. There were no treatment-related changes in intrauterine survival and fetal weight, and no changes in the incidence of developmental malformations and variations compared to controls Parental toxicity: NOAEL >1,000 mg/kg bw-day (highest dose tested Reproductive toxicity: NOAEL >1,000 mg/kg bw-day (highest dose tested	NIEHS 1999; IUCLID 2000; HPV 2008	Reported in secondary sources; sufficient study details provided. The study is in accordance with OPPTS method 870.3700; only one dose level tested.
	Postnatal Development			No data located.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Neurotoxicity		**MODERATE: There is potential for neurobehavioral effects estimated based on analogy to decabromodiphenyl ether and professional judgment.**		
	Neurotoxicity Screening Battery (Adult)	Mice as neonates (day 3, 10, 19), single oral dose; neurobehavioral effects (Estimated by analogy)	Professional judgment	Estimated based on analogy to decabromodiphenyl ether.
Repeated Dose Effects		**LOW: A 28- or 90-day dietary exposure to ethylene bis-tetrabromophthalimide in rats at doses as high as 1,000 mg/kg bw-day did not cause adverse effects on growth parameters, clinical chemistry, organ weights and weight ratios, or macro and micro pathology. By analogy to decabromodiphenyl ether and with the potential for bioaccumulation, there is potential for expression of adverse effects in longer term studies.**		
		Potential for repeated dose effects (Estimated by analogy and bioaccumulation)	Professional judgment	Estimated based on the high potential for bioaccumulation and by analogy to observations on decabromodiphenyl ether where adverse effects were not present in 90-day studies but were expressed following chronic exposure in a NTP study.
		In a 28-day oral (dietary) study in male rats (10/group) fed 0, 0.01, 0.1, or 1% ethylene bis-tetrabromophthalimide, there were no treatment-related changes in growth parameters or food consumption, clinical chemistry, terminal organ weights or weight ratios, or gross and microscopic tissues. NOAEL >1% in diet (> 1,000 mg/kg-bw-day) (highest dose tested)	NIEHS 1999; IUCLID 2000; HPV 2008	Reported in a secondary source; sufficient study details provided. The study does not conform to current guidelines.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		In a 90-day oral (dietary) study in rats fed 0, 0.01, 0.1, or 1% ethylene bis-tetrabromophthalimide, there were no treatment-related changes in growth parameters or food consumption, clinical chemistry, terminal organ weights or weight ratios, or gross and microscopic tissues; there were unspecified changes in urinalysis. NOAEL >1% in diet (> 1,000 mg/kg bw-day) (highest dose tested)	NIEHS 1999; IUCLID 2000; HPV 2008	Reported in a secondary source; sufficient study details provided. The study does not conform to current guidelines.
Skin Sensitization		**LOW: Estimated to have Low potential for skin sensitization based on expert judgment.**		
	Skin Sensitization	Low potential for skin sensitization.	Expert judgment	Estimated based on expert judgment.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**VERY LOW: Ethylene bis-tetrabromophthalimide is not an eye irritant.**		
	Eye Irritation	Not irritating, New Zealand white rabbit	NIEHS 1999; IUCLID 2000	Reported in a secondary source; some study details provided.
		Not irritating, albino rabbit	IUCLID 2000	Reported in a secondary source; limited study details provided.
Dermal Irritation		**VERY LOW: Ethylene bis-tetrabromophthalimide is not a skin irritant.**		
	Dermal Irritation	Not irritating, rabbit; 24-hour occlusive dressing.	IUCLID 2000	Reported in a secondary source; limited study details provided.
		Not irritating, rabbit; 24-hour abraded and nonabraded sites; 24-hour occlusive dressing	NIEHS 1999; IUCLID 2000	Reported in secondary sources; sufficient study details provided.
Endocrine Activity		**No data located.**		
				No data located.
Immunotoxicity		**Estimated to have no potential for immunotoxicity based on expert judgment.**		
	Immune System Effects	Expected to not have potential for immunotoxicity. (Estimated)	Expert judgment	Estimated based on expert judgment.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
ECOTOXICITY			
ECOSAR Class	Imides; Amides		
Acute Toxicity	**LOW: Estimated data suggest no effects at saturation (NES) for the acute aquatic toxicity endpoints; experimental results are too short a duration to assess the hazard of acute aquatic toxicity, but are consistent with this hazard designation.**		
Fish LC_{50}	*Oryzias latipes* (orange-red killifish) 48-hour LC_{50} > 500 mg/L (static) (Experimental)	NIEHS 1999; IUCLID 2000; HPV 2008	48-hour exposure study as opposed to preferred 96-hour study; according to MITI guidelines.
	Fish 96-hour LC_{50} = 0.000084 mg/L (Estimated) ECOSAR: Amides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Fish 96-hour LC_{50} = 0.00022 mg/L (Estimated) ECOSAR: Imides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Fish 96-hour LC_{50} = 0.00019 mg/L (Estimated) ECOSAR: neutral organics	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Daphnid LC_{50}	Daphnid 48-hour LC_{50} = 0.000274 mg/L (Estimated) ECOSAR: Neutral organic	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Daphnid 48-hour LC_{50} = 0.000469 mg/L (Estimated) ECOSAR: Imides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Daphnid 48-hour LC_{50} = 0.000695 mg/L (Estimated) ECOSAR: Amides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
Green Algae EC_{50}	Green algae 96-hour EC_{50} = 0.003 mg/L (Estimated) ECOSAR: Neutral organic	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
	Green algae 96-hour EC_{50} = 0.02 mg/L (Estimated) ECOSAR: Imides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
	Green algae 96-hour EC_{50} = 0.014 mg/L (Estimated) ECOSAR: Amides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
Chronic Aquatic Toxicity	**LOW: Estimated data suggest NES for chronic aquatic toxicity endpoints.**		
Fish ChV	Fish 30-day ChV = 0.000000494 mg/L (Estimated) ECOSAR: Amides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
	Fish 30-day ChV = 0.0000196 mg/L (Estimated) ECOSAR: Imides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Fish 30-day ChV = 0.0000148 mg/L (Estimated) ECOSAR: Neutral organics	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
Daphnid ChV	Daphnid ChV = 0.00000917 mg/L (Estimated) ECOSAR: Amides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
	Daphnid ChV = 0.000115 mg/L (Estimated) ECOSAR: Imides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
	Daphnid ChV = 0.000101 mg/L (Estimated) ECOSAR: Neutral organics	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
Green Algae ChV	Green algae ChV = 0.004 mg/L (Estimated) ECOSAR: Neutral organic	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
	Green algae ChV = 0.008 mg/L (Estimated) ECOSAR: Imides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
	Green algae ChV = 1.59 mg/L (Estimated) ECOSAR: Amides	EPI	NES: The log K_{ow} of 9.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**The transport evaluation for ethylene bis-tetrabromophthalimide is based on estimated physical and chemical properties. Based on the Level III fugacity models incorporating the located experimental property data, ethylene bis-tetrabromophthalimide is expected to partition primarily to soil. It is not expected to dissociate at environmentally-relevant pH. Ethylene bis-tetrabromophthalimide is expected to have low mobility in soil based on its estimated K_{oc}. Therefore, leaching of ethylene bis-tetrabromophthalimide through soil to groundwater is not expected to be an important transport mechanism. Estimated volatilization half-lives indicate that it will be non-volatile from surface water. In the atmosphere, ethylene bis-tetrabromophthalimide is expected to exist in the particulate phase, based on its estimated vapor pressure. Particulates will be removed from air by wet or dry deposition.**		
	Henry's Law Constant (atm-m^3/mole)	<10^{-8} (Estimated)	EPI; Professional judgment	Cutoff value for non volatile compounds.
	Sediment/Soil Adsorption/ Desorption Coefficient – K_{oc}	>30,000 (Estimated)	EPI; EPA, 2011	Cutoff value for non mobile compounds according to SF assessment guidance.
	Level III Fugacity Model	Air ≤ 1% Water = 5.4% Soil = 95% Sediment ≤ 1%	EPI	
Persistence		**VERY HIGH: The very high persistence concern for ethylene bis-tetrabromophthalimide is based on limited experimental data and QSAR estimates. No degradation observed in activated sludge during a Japanese MITI test, indicating it is not biodegradable under the stringent test conditions. Results from biodegradation models provided similar results and indicate that it will be recalcitrant under aerobic conditions. Anaerobic degradation under methanogenic conditions is not considered probable. The atmospheric half-life of ethylene bis-tetrabromophthalimide is estimated to be 3.3 hours, although it is expected to exist primarily in the particulate phase in air. Resistance to most environmental fate processes indicates that ethylene bis-tetrabromophthalimide is expected to be persistent in the environment.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Primary and Ultimate Survey Model)	EPI	
	Volatilization Half-life for Model River	>1 year (Estimated)	EPI	

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Volatilization Half-life for Model Lake	>1 year (Estimated)	EPI	
Soil	**Aerobic Biodegradation**	0% after 28 days Japanese MITI test (Measured)	HPV, 2008	Guideline study reported in a secondary source.
	Anaerobic Biodegradation	Not probable (Anaerobic-methanogenic biodegradation probability model)	EPI	
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	3.3 hours	EPI	
Reactivity	**Photolysis**			No data located.
	Hydrolysis			No data located.
Environmental Half-life		>180 days (Estimated)	EPI; PBT Profiler	Half-life estimated for the predominant compartment, as determined by EPI and the PBT Profiler methodology.
Bioaccumulation		**HIGH: The potential for bioaccumulation of ethylene bis-tetrabromophthalimide is high based on the estimated BAF. When a single BCF measurement is available DfE assessment criteria indicate that estimated BAF values are used in a conservative approach. The BAF estimate is consistent with that anticipated for high MW chemicals with a high degree of bromination.**		
	Fish BCF	<0.3 - <3 (Measured) in Japanese carp using OECD Test Guideline 305C	Hardy, 2004	Adequate guide line study reported in a secondary source.
	BAF	1.7×10^{5} (Estimated)	EPI	
	Metabolism in Fish			No data located.

Ethylene Bis-Tetrabromophthalimide CASRN 32588-76-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL MONITORING AND BIOMONITORING			
Environmental Monitoring	No data located.		
Ecological Biomonitoring	No data located.		
Human Biomonitoring	This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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Magnesium Hydroxide

Screening Level Hazard Summary

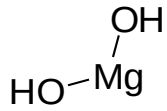
This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

[R] Recalcitrant: Substance is comprised of metallic species that will not degrade, but may change oxidation state or undergo complexation processes under environmental conditions

		Human Health Effects											Aquatic Toxicity		Environmental Fate	
Chemical	CASRN	Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Magnesium Hydroxide	1309-42-8	L	L	L	*L*	*L*	*L*	L	*L*		M	*M*	*L*	*L*	*H*[R]	*L*

Magnesium Hydroxide

<table>
<tr><td rowspan="5">  </td><td>CASRN: 1309-42-8</td></tr>
<tr><td>MW: 58.32</td></tr>
<tr><td>MF: MgH_2O_2</td></tr>
<tr><td>Physical Forms:
Neat: Solid</td></tr>
<tr><td>Use: Flame retardant</td></tr>
<tr><td colspan="2">SMILES: O[Mg]O</td></tr>
<tr><td colspan="2">Synonyms: Magnesium hydroxide (Mg(OH)2) (TSCA Inventory); Brucite, Milk of Magnesia; Alcanex NHC 25, Asahi Glass 200-06, Baschem 12, Combustrol 500, Duhor, Duhor N, Ebson RF, FloMag H, FloMag HUS, Hydro-mag MA, Hydrofy G 1.5, Hydrofy G 2.5, Hydrofy N, Kisuma 4AF, Kisuma 5, Kisuma 5A, Kisuma 5B, Kisuma 5B-N, Kisuma 5BG, Kisuma 5E, Kisuma 78, Kisuma S 4, Kyowamag F, Lycal 96 HSE, Mag Chem MH 10, Magmesia hydrate, MagneClear 58, Magnesia magma, Magnesiamaito, Magnesium dihydroxide, Magnesium hydroxide gel, Magnesium(II) hydroxide, Magnifin H 10, Magox, Marinco H, Marinco H 1241, Martinal VPF 8812, Milmag, Mint-O-Mag, Nemalite, Oxaine M, Phillips Magnesia Tablets, Phillips Milk of Magnesia Liquid, Reachim, Star 200, Versamag</td></tr>
<tr><td colspan="2">Chemical considerations: This alternative is an inorganic compound. In the absence of experimental data, professional judgment using chemical class and structural considerations were used to complete this hazard profile.</td></tr>
<tr><td colspan="2">Polymeric: No
Oligomers: Not applicable</td></tr>
<tr><td colspan="2">Metabolites, Degradates and Transformation Products: Not applicable</td></tr>
<tr><td>Analog: No analogs; Mg^{2+} ions are expected to form when $Mg(OH)_2$ and other magnesium containing compounds dissociate in aqueous conditions. Studies included in this assessment demonstrate the hazards associated with Mg^{2+} from other sources like $MgCl_2$.
Endpoint(s) using analog values: Not applicable</td><td>Analog Structure: Not applicable</td></tr>
<tr><td colspan="2">Structural Alerts: None</td></tr>
<tr><td colspan="2">Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).</td></tr>
<tr><td colspan="2">Hazard and Risk Assessments: Risk assessment completed for magnesium hydroxide by the National Academy of Sciences in 2000 (NAS, 2000).</td></tr>
<tr><td colspan="2">U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory</td></tr>
</table>

Magnesium Hydroxide CASRN 1309-42-8			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	Decomposes at 350 (Measured)	Hodgman, 1959; Lewis, 1997; Lewis, 2000	MgO and H_2O are decomposition products.
	Decomposes at 380 (Measured)	IUCLID, 2000	
	350 (Measured)	Lide, 2000; Aldrich, 2006	
Boiling Point (°C)	Will decompose before boiling (Measured)	IUCLID, 2000	Decomposition occurs upon melting as described in additional sources above.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2011	Cutoff value for nonvolatile compounds according to SF assessment guidance. This inorganic compound is not amenable to available estimation methods.
Water Solubility (mg/L)	1.78 at 20°C, pH 8.3 (Measured) According to OECD 105 column elution method.	ECHA, 2010	Guideline study; results are in agreement with other experimental values.
	9 at 18°C (Measured)	Hodgman, 1959; IUCLID, 2000	Measured values, which span a relatively narrow range, are consistently reported in numerous sources.
	1 at 20°C (Measured)	IUCLID, 2000	
	6 at 20°C (Measured)	IUCLID, 2000	
	<8 at 20°C (Measured)	IUCLID, 2000	
	40 at 100°C (Measured)	Hodgman, 1959	Value obtained at an elevated temperature.
Log K_{ow}			No data located; inorganic compounds are outside the estimation domain of EPI.
Flammability (Flash Point)	Not flammable (Estimated)	IUCLID, 2000	Adequate.
Explosivity	Not explosive (Estimated)	IUCLID, 2000	Adequate.

Magnesium Hydroxide CASRN 1309-42-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Pyrolysis		Not applicable (Estimated)	Professional judgment	Inorganic compounds do not undergo pyrolysis.
pH		9.5-10.5 (Measured)	O'Neil et al., 2011	Adequate.
		pH of a saturated solution in water was 8.3 (Measured)	ECHA, 2010	Reported in a secondary source, determined from a water solubility study.
pK_a				No data located; inorganic compounds are outside the estimation domain of the SPARC model.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Some magnesium hydroxide is absorbed following ingestion and is excreted primarily in urine.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	The magnesium ion is poorly absorbed; when taken orally, only 5-15% of the magnesium from a dose of magnesium hydroxide is absorbed and this magnesium is readily excreted in the urine, if kidney function is normal.	IUCLID, 2000	Reported in a secondary source, limited study details provided.
Acute Mammalian Toxicity		**LOW: Acute lethality values suggest that magnesium hydroxide is of low concern for acute toxicity for oral exposure. There were no data located regarding acute dermal and inhalation exposure.**		
Acute Lethality	**Oral**	Rat oral LD_{50} = 8,500 mg/kg-bw	Lewis, 2000	Reported in a secondary source, limited study details provided.
		Mouse oral LD_{50} = 8,500 mg/kg-bw	Lewis, 2000	Reported in a secondary source, limited study details provided.
		Human infant oral TD_{Lo} (behavioral) = 2,747 mg/kg	Lewis, 2000	Reported in a secondary source, limited study details provided.
		Probable human oral lethal dose = 5-15 g/kg-bw	HSDB, 2008	Reported in a secondary source, limited study details provided.
	Dermal			No data located.
	Inhalation	Rat inhalation LC_{50} > 2.1 mg/L	ECHA, 2010	Reported in a secondary source. There was no mortality at the highest dose tested (2.1 mg/L).

Magnesium Hydroxide CASRN 1309-42-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Carcinogenicity		**LOW: Experimental studies indicate that magnesium hydroxide is of low concern for carcinogenicity.**		
	OncoLogic Results			Structure could not be evaluated by OncoLogic.
	Carcinogenicity (Rat and Mouse)	5-week, repeated-dose/carcinogenicity study, oral (diet), rat; Decreased number of carcinogen-induced DNA synthesis in the large bowel epithelial cells. NOAEL >2,000 ppm (approximately 100 mg/kg/day, highest dose tested)	BIBRA, 1993	Reported in a secondary source, limited study details provided.
	Combined Chronic Toxicity/ Carcinogenicity	96-week chronic toxicity/carcinogenicity study on $MgCl_2$, oral, mouse; no significant differences in tumor incidence between treated and control animals except for dose-related decrease in the incidence of hepatocellular carcinomas in males.	Kurata et al., 1989	Sufficient study details reported in a primary source.
		227-day, chronic toxicity/ carcinogenicity study, oral (diet), rat; decreased number of colon tumors in rats pretreated with a known colon carcinogen. NOAEL >50 mg/kg/day (highest dose tested)	BIBRA, 1993	Reported in a secondary source, limited study details provided.
		16-week carcinogenicity study, oral (diet), rat; inhibitory effects on colon carcinogenesis, carcinogen-induced expression of *c-myc* proto-oncogene and cell proliferation. NOAEL = 0.2%in diet (highest concentration tested)	Wang et al., 1993	Sufficient study details reported in a primary source.

Magnesium Hydroxide CASRN 1309-42-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Inhalation exposure of male rats to short (4.9 x 0.31 mm) or long (12 x 0.44 mm) $MgSO_4/5Mg(OH)_2\ 3H_20$ filaments for 6 hour/day, 5 day/week for up to 1 year did not increase the incidence of any tumor types in animals sacrificed 1 day or 1 year after cessation of exposure.	NAS, 2000	Reported in a secondary source, limited study details provided.
Genotoxicity		**LOW: Experimental studies indicate that magnesium hydroxide is not mutagenic to bacteria or mammalian cells *in vitro* and does not cause chromosomal aberrations in human lymphocytes *in vitro* .**		
	Gene Mutation *in vitro*	Negative, Ames Assay in *Salmonella* and *Escherichia coli*	BIBRA, 1993	Reported in a secondary source, limited study details provided. Only 3 strains of *Salmonella* were tested; current regulatory guidelines suggest that at least 4 strains be used in Ames tests.
		Negative; mouse lymphoma assay, L5178Y cells; with and without metabolic activation	ECHA, 2010	Reported in a secondary source.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	Negative; did not induce chromosomal aberrations in human lymphocytes; with and without metabolic activation	ECHA, 2010	Reported in a secondary source.
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: Magnesium hydroxide is expected to be of low concern for reproductive effects based on a nonstandard experimental study indicating magnesium chloride produces no adverse effects on reproductive performance or outcomes at levels up to 96 mg/kg/day of Mg^{2+} ion. In addition, there were no reproductive effects observed in rats in a repeated dose toxicity study with the reproduction/developmental toxicity screen at doses as high as 1,000 mg/kg-day.**		

Magnesium Hydroxide CASRN 1309-42-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Reproduction/ Developmental Toxicity Screen	10-day (GD 6-15) reproductive/developmental study on $MgCl_2$, oral, rat; no maternal or reproductive effects. NOAEL >96 mg/kg/day for Mg^{2+} ion (highest dose tested)	NAS, 2000	Reported in a secondary source, limited study details provided.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	Repeated dose toxicity study with the reproduction/developmental toxicity screen; rat, oral (gavage), 0, 110, 330, 1000 mg/kg-day. Males exposed for 29 days: 2 weeks prior to mating, during mating and up to termination; females exposed for 41-45 days: 2 weeks premating, during mating, post coitum, and 4 days of lactation. There were no reproductive effects observed in any dose group. NOAEL = > 1,000 mg/kg-day LOAEL = Not established	ECHA, 2010	Reported in a secondary source. Study conducted according to OECD 422.
	Reproduction and Fertility Effects			No data located.

Magnesium Hydroxide CASRN 1309-42-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**LOW: Magnesium hydroxide is expected to be of low concern for developmental effects based on weight a nonstandard experimental study indicating magnesium chloride produces no adverse effects on developmental outcomes at levels up to 96 mg/kg/day of Mg^{2+} ion and an experimental study from a secondary source showing no effect on human newborns. In addition, there were no developmental effects observed in rats in a repeated dose toxicity study with the reproduction/developmental toxicity screen at doses as high as 1,000 mg/kg-day.**		
	Reproduction/ Developmental Toxicity Screen	10-day (GD 6-15) reproductive/developmental study on $MgCl_2$, oral, rat; no maternal or reproductive effects. NOAEL >96 mg/kg/day for Mg^{2+} ion (highest dose tested)	NAS, 2000	Reported in a secondary source, limited study details provided.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	Repeated-dose/developmental study (fetal exposure at unspecified dose levels during 3rd trimester), 27 hypertensive women treated with magnesium hydroxide, no effect on newborns except slightly increased body weight and hypermagnesiumemia. Cord serum Mg levels reported to be 70-100% of maternal levels after treatment (potentially causing neurological depression in neonate, characterized by respiratory depression, muscle weakness, decreased reflexes). Prolonged magnesium treatment during pregnancy may be associated with maternal and fetal hypocalcemia and adverse effects on fetal bone mineralization.	HSDB, 2008	Reported in a secondary source, limited study details provided. Maternal treatment doses not specified.

Magnesium Hydroxide CASRN 1309-42-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Repeated dose toxicity study with the reproduction/developmental toxicity screen; rat, oral (gavage), 0, 110, 330, 1000 mg/kg-day. Males exposed for 29 days: 2 weeks prior to mating, during mating and up to termination; females exposed for 41-45 days: 2 weeks premating, during mating, post coitum, and 4 days of lactation. There were no developmental effects observed in any dose group. NOAEL = > 1,000 mg/kg-day LOAEL = Not established	ECHA, 2010	Reported in a secondary source. Study conducted according to OECD 422.
	Prenatal Development			No data located.
	Postnatal Development			No data located.
Neurotoxicity		**LOW: Magnesium hydroxide is expected to be of low hazard for neurotoxicity based on expert judgment.**		
	Neurotoxicity Screening Battery (Adult)	Low potential for neurotoxicity. (Estimated)	Expert judgment	Estimated based on expert judgment.

Magnesium Hydroxide CASRN 1309-42-8			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects	**LOW: Experimental studies indicate magnesium ions produce no adverse systemic effects in rats or mice at magnesium levels ≥1,000 mg/kg/day of magnesium hydroxide.**		
	96-week repeated-dose study for $MgCl_2$, oral, mouse; decreased body weight gain, increased food/water consumption and increased relative brain, heart and kidney weights in high dose females, no effects in males. Female: LOAEL = 470 mg/kg/day for Mg^{2+} ion NOAEL = 87 mg/kg-day for Mg^{2+} ion Male: NOAEL = 336 mg/kg-day for Mg^{2+} ion (highest dose tested) LOAEL = not established	Kurata et al., 1989	Adequate, primary source.
	90-day repeated-dose study for $MgCl_2$, oral, mouse; decreased body weight gain in males and females at highest doses tested; renal tubular vacuolation in males administered 650 mg/kg/day for Mg^{2+} ion. Female: LOAEL = 1,660 mg/kg/day for Mg^{2+} ion NOAEL = 817 mg/kg/day for Mg^{2+} ion Male: LOAEL = 650 mg/kg/day for Mg^{2+} ion NOAEL = 322 mg/kg/day for Mg^{2+} ion	NAS, 2000	Reported in a secondary source, no study details provided.

Magnesium Hydroxide CASRN 1309-42-8			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	90-day repeated-dose study for $MgCl_2$, oral, mouse; decreased body weight gain, renal tubular vacuolation in males. Female: NOAEL = 587 mg/kg/day for Mg^{2+} ion Male: LOAEL = 840 mg/kg-day NOAEL = 420 mg/kg/day for Mg^{2+} ion	NAS, 2000	Reported in a secondary source, no study details provided.
	32-week repeated-dose study, diet, rat; no effects on body weight or liver weight. NOAEL >1,000 ppm (approximately 50 mg/kg/day)	BIBRA, 1993	Reported in a secondary source, no study details provided.
	Inhalation exposure of male rats to short (4.9 x 0.31 mm) or long (12 x 0.44 mm) $MgSO_4/5Mg(OH)_2 \cdot 3H_2O$ filaments for 6 hour/day, 5 day/week for up to 1 year (concentration not specified) exhibited a slight increase in the incidence of pulmonary lesions 1 year after cessation of exposure. Histopathological examination revealed a slight increase in segmental calcification of the pulmonary artery and thickening of the lung pleura in rats exposed to both short and long filaments for 4 weeks or 1 year. There were no effects on survival or body, lung, liver, kidney and spleen weights of animals sacrificed 1 day or 1 year following a 1-year exposure period.	NAS, 2000	Reported in a secondary source, no study details provided.

Magnesium Hydroxide CASRN 1309-42-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		4-week repeated-dose study, oral, human; caused diarrhea, abdominal discomfort, and increased serum magnesium levels. LOAEL = 400 mg/day	BIBRA, 1993	Reported in a secondary source, no study details provided.
		Repeated dose toxicity study with the reproduction/developmental toxicity screen; rat, oral (gavage), 0, 110, 330, 1000 mg/kg-day. Males exposed for 29 days: 2 weeks prior to mating, during mating and up to termination; females exposed for 41-45 days: 2 weeks premating, during mating, post coitum, and 4 days of lactation. There were no toxicologically relevant changes in any of the parental parameters examined. NOAEL = > 1,000 mg/kg-day LOAEL = Not established	ECHA, 2010	Reported in a secondary source. Study conducted according to OECD 422.
		Human systemic effects: chlorine level changes, coma, somnolence.	Lewis, 2000	Reported in a secondary source, no study details provided.
		Repeated use in humans may rarely cause rectal stones composed of magnesium carbonate and magnesium hydroxide.	IUCLID, 2000	Reported in a secondary source, no study details provided.
Skin Sensitization		**LOW: Magnesium hydroxide is not estimated to cause skin sensitization based on professional judgment.**		
	Skin Sensitization	Does not cause skin sensitization (Estimated)	Professional judgment	Estimated by professional judgment.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**MODERATE: Based on irritation and damage to the corneal epithelium in rabbits that cleared within 2-3 days.**		

Magnesium Hydroxide CASRN 1309-42-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Eye Irritation	Moderately irritating to rabbit eyes.	IUCLID, 2000	Reported in a secondary source, limited study details provided.
		Administration of milk of magnesia twice a day for 3-4 days caused damage to corneal epithelium of rabbit eyes; however, effects disappeared within 2-3 days.	HSDB, 2008	Reported in a secondary source, limited study details provided. Milk of magnesia is a mixture containing magnesium hydroxide and inactive ingredients.
Dermal Irritation		**MODERATE: Magnesium hydroxide is expected to have moderate potential for dermal irritation based on expert judgment considering the basicity of a saturated aqueous solution and a secondary source indicating that it causes skin irritation.**		
	Dermal Irritation	Moderate potential for dermal irritation based on experimental aqueous pH values. (Estimated)	Expert judgment	Estimated based on expert judgment.
		Causes skin irritation	Fisher Scientific, 2007	Reported in a secondary source, no experimental study was identified or study details provided.
		Not corrosive in an *in vitro* human skin corrosion test.	ECHA, 2010	Reported in a secondary source. Study conducted according to OECD guideline 431.
		Not irritating in an *in vitro* skin irritation test.	ECHA, 2010	Reported in a secondary source. *In vitro* skin irritation: reconstructed human epidermis model test.
Endocrine Activity		**No data located.**		
				No data located.
Immunotoxicity		**Magnesium hydroxide is expected to be of low hazard for immunotoxicity based on expert judgment.**		
	Immune System Effects	Low potential for immunotoxicity. (Estimated)	Expert judgment	Estimated based on expert judgment.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**LOW: Estimated LC_{50} values for all of the species in the standard toxicity profile are greater than 100 mg/L. LC_{50} values are much greater than the anticipated water solubility, suggesting no effects at saturation (NES).**		

Magnesium Hydroxide CASRN 1309-42-8			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Fish LC_{50}	96-hour LC_{50} = 1,110 mg/L (Estimated)	Mount et al., 1997	Estimated from the measured LC_{50}s for $MgCl_2$ and $MgSO_4$, modified by a MW adjustment for $Mg(OH)_2$; expected to display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.
	Pimephalis promelas 96-hour LC_{50} = 511 mg/L; static conditions (Experimental)	ECHA, 2010	Reported in a secondary source. Test material diluted to 61% in aqueous suspension.
	Onchorinchus mykiss 96-hour LC_{50} = 775.8 mg/L; static conditions (Experimental)	ECHA, 2010	Reported in a secondary source. Test material diluted to 61% in aqueous suspension.
Daphnid LC_{50}	48-hour LC_{50} = 648 mg/L (Estimated)	Biesinger and Christensen, 1972; Mount et al., 1997	Estimated from the measured LC_{50}s for $MgCl_2$ and $MgSO_4$, modified by a MW adjustment for $Mg(OH)_2$; expected to display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.
	Daphnia magna 48-hour LC_{50} = 284.76 mg/L; static conditions (Experimental)	ECHA, 2010	Reported in a secondary source. Test material diluted to 61% in aqueous suspension.
Other Freshwater Invertebrate LC_{50}	*Gammarus lacustris* LC_{50} = 64.7 mg/L (Experimental)	O'Connell et al., 2004	Reported in a secondary source, study details and test conditions were not provided. Not a standard test species.
Green Algae EC_{50}	96-hour EC_{50} = 2,111 mg/L (Estimated)	Professional judgment	Estimated using an acute to chronic ratio of 4; expected to display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.

Magnesium Hydroxide CASRN 1309-42-8			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Scenedesmus subspicatus and Delenastrum capricornutum 72-hour EC_{50} > 100 mg/L (for growth and biomass) (Experimental)	ECHA, 2010	Reported in a secondary source.
Chronic Aquatic Toxicity	**LOW: Estimated chronic values (ChV) are all >10 mg/L. ChVs are much greater than the anticipated water solubility, suggesting NES.**		
Fish ChV	403 mg/L (Estimated)	Professional judgment	Estimated using an acute to chronic ratio of 3:3; expected to display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.
Daphnid ChV	197 mg/L (Estimated)	Suter, 1996	Estimated from the measured ChV for Mg^{2+} ion, modified by a MW adjustment for $Mg(OH)_2$; expected to display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.
Green Algae ChV	528 mg/L (Estimated)	ECOTOX database	Estimated from the measured NOEC and LOEC for $MgSO_4$, modified by a MW adjustment for $Mg(OH)_2$; expected to display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.
ENVIRONMENTAL FATE			
Transport	**The low water solubility, the estimated vapor pressure of <1x10^{-8} mm Hg, estimated K_{oc} of >30,000 and estimated Henry's Law Constant of <1x10^{-8} atm-m^3/mole indicate that magnesium hydroxide will be relatively immobile in the environment. Magnesium hydroxide is a mineral occurring naturally in the environment.**		

Magnesium Hydroxide CASRN 1309-42-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment	Cutoff value for nonvolatile compounds. This inorganic compound is not amenable to available estimation methods.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; U.S. EPA, 2011	Cutoff value for nonmobile compounds according to SF assessment guidance. This inorganic compound is not amenable to available estimation methods.
	Level III Fugacity Model			Not all input parameters for this model were available to run the estimation software (EPI).
Persistence		**HIGH: As an inorganic compound, magnesium hydroxide is not expected to biodegrade, oxidize in air, or undergo hydrolysis under environmental conditions. Magnesium hydroxide does not absorb light at environmentally relevant wavelengths and is not expected to photolyze. Magnesium hydroxide is recalcitrant and it is expected to be found in the environment >180 days after release. As a naturally occurring compound, it may participate in natural cycles and form complexes in environmental waters.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment	Substance is or contains inorganic elements, such as metal ions or oxides, that are expected to be found in the environment >180 days after release.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
Soil	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment	This inorganic compound is not amenable to available estimation methods.
	Anaerobic Biodegradation	Recalcitrant (Estimated)	Professional judgment	This inorganic compound is not amenable to available estimation methods.

Magnesium Hydroxide CASRN 1309-42-8				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	>1 year (Estimated)	Professional judgment	Substance does not contain functional groups amenable to atmospheric degradation processes.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Professional judgment	Magnesium hydroxide does not absorb UV light at environmentally relevant wavelengths and is not expected to undergo photolysis.
	Hydrolysis	Not a significant fate process (Estimated)	Professional judgment	Substance does not contain functional groups amenable to hydrolysis.
Environmental Half-life				Not all input parameters for this model were available to run the estimation software (EPI).
Bioaccumulation		**LOW: Magnesium hydroxide is not expected to bioaccumulate based on professional judgment.**		
	Fish BCF	<100 (Estimated)	Professional judgment	This inorganic compound is not amenable to available estimation methods.
	BAF	<100 (Estimated)	Professional judgment	This inorganic compound is not amenable to available estimation methods.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		Magnesium hydroxide is a mineral that occurs naturally in the environment.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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Melamine Cyanurate

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with a substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

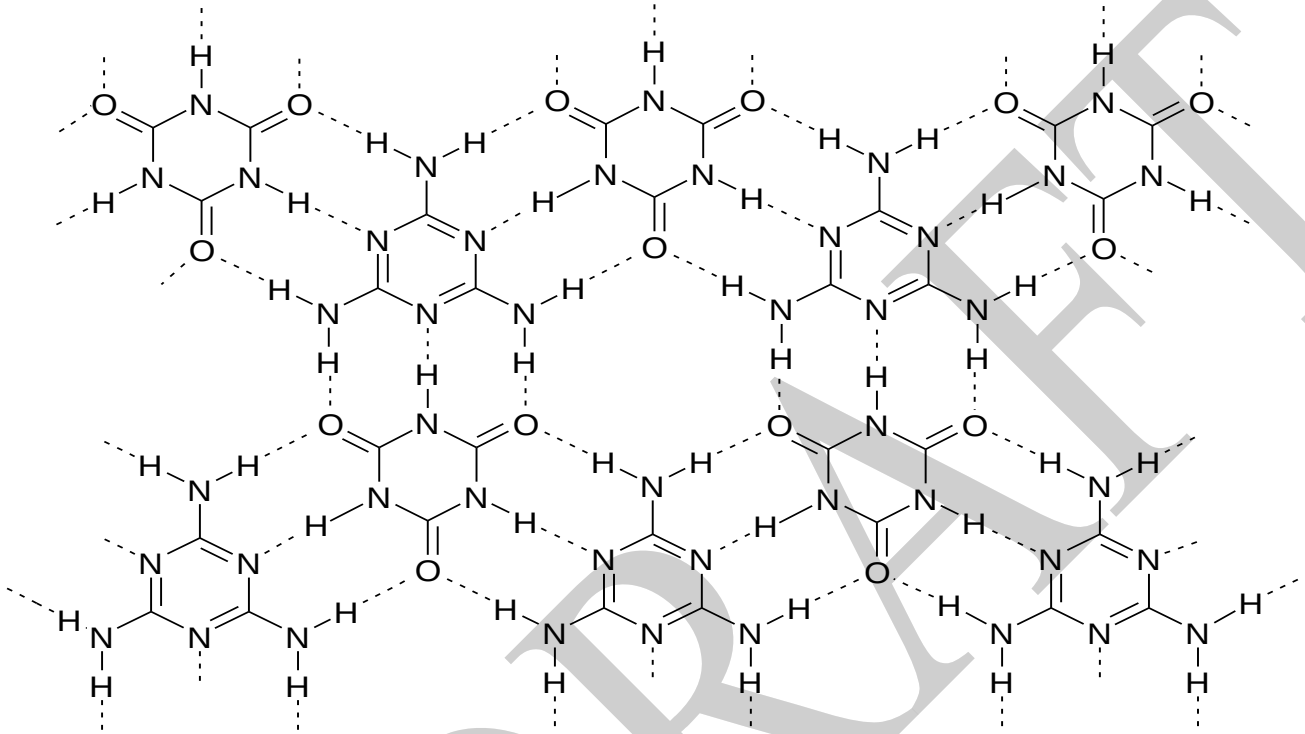
VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from estimation software and professional judgment.

§ Based on analogy to experimental data for a structurally similar compound.

Chemical	CASRN	Human Health Effects										Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Melamine Cyanurate[1]	37640-57-6	*L*	*M*	*M*	*M*§	*M*§	*L*	H	*L*		*L*	*L*	*L*	L	VH	*L*

[1] Hazard designations are based upon the component of the salt with the highest hazard designation, including the corresponding free acid or base.

Melamine Cyanurate



CASRN: 37640-57-6

MW: 255 (Empirical)

MF: $C_3H_6N_6 \cdot C_3H_3N_3O_3$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: n1c(N)nc(N)nc1N(H)(H)(H)N2C(=O)NC(=O)NC2=O (Empirical)

Synonyms: 1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, compd. with 1,3,5-triazine-2,4,6-triamine (1:1) (TSCA Inventory); 1,3,5-triazinane-2,4,6-trione - 1,3,5-triazine-2,4,6-triamine (1:1); Melapur MC XL; Melamine isocyanurate

Chemical Considerations: This alternative is an organic salt of melamine (CASRN 108-78-1) and cyanuric acid (CASRN 108-80-5) organized in a well ordered crystalline complex, with extensive intramolecular hydrogen bonding. The abundance of complimentary hydrogen bonds effectively link melamine and cyanuric acid into stable lattice chains. The potential for dissolution of these chains are dependent on pH. The simplest 1:1 melamine cyanurate complex has an empirical molecular weight of 255; although higher molecular weight networks are expected because the integrated melamine cyanurate complex has a higher degree of stabilization than isolated components (Perdigáo, 2006). This assessment will consider the worst case hazard concerns which may include those from the dissolution of melamine and cyanuric acid from the complex.	
Polymeric: No **Oligomers:** Not applicable	
Metabolites, Degradates and Transformation Products: Melamine (CASRN 108-78-1); cyanuric acid (CASRN 108-80-5)	
Analogs: Confidential analog, nitrogen heterocycles **Endpoint(s) using analog values:** Reproductive Effects, Development Effects	**Analog Structures:** Confidential; nitrogen heterocycles is a class of cyclic compounds that have nitrogen atoms and at least one other element as members of its ring.
Structural Alerts: Aromatic amine (U.S. EPA, 2011a)	
Risk Phrases: Xn- harmful; R48/22 - harmful: danger of serious damage to health by prolonged exposure if swallowed (ECHA, 2011a).	
Hazard and Risk Assessments: None identified	
U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory and is a commenced Premanufacture Notice substance.	

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)			No data located.
Boiling Point (°C)	>350 decomposes (Measured)	Leisewitz et al., 2001; ECHA, 2011a	Based on the reported thermal stability value.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2011b	Cutoff value for non volatile compounds according to SF assessment guidance; based on the ionic nature of the material.
Water Solubility (mg/L)	Approximately 27 at 20°C (OECD 105) (Measured)	ECHA, 2011a	Guideline study.
	10 at 20°C (Measured)	ECHA, 2011a	Non-guideline studies at neutral pH that substantiate the limited solubility anticipated under neutral conditions.
	1 at 20°C (Measured)	ECHA, 2011a	
	2 at 25°C (Measured)	Ciba, 2001	
	1.5 at 37°C (Measured)	ECHA, 2011a	
	Under neutral conditions melamine and cyanuric acid form a stable and insoluble hydrogen-bonded network; the network is destabilized at pH extremes (Measured)	Rovner, 2008	Non-quantitative supporting information that describes the behavior of the compound in water.
	Very insoluble in water (Measured)	Crews, 2006	Inadequate; qualitative, nonspecific Value.
	Not soluble at room temperature (Measured)	ICL Industrial Products (IP), 2011	
Log K_{ow}	**Melamine Cyanurate:** < 0 (Estimated) **Melamine:** -1.37 (Measured) **Cyanuric Acid:** -0.47 (Measured)	ECHA, 2011a; Hansch, 1995; Kaune et al., 1998; Pakalin et al., 2007	Inadequate, based on experimental water solubility data. These values are not applicable for the melamine cyanurate complex.
Flammability (Flash Point)	Self-ignition temperature: >400°C (Measured)	ECHA, 2011a	Adequate.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
pH	5-6 (Measured)	ECHA, 2011a	Inadequate, these data are not consistent with the well conducted water solubility studies; purity of test material not reported.
	5.5 (Measured)	Ciba, 2001	
pK_a	**Melamine:** 5 (Measured) **Cyanuric Acid:** 6.88, 11.4, 13.5 (Measured)	ECHA, 2011a	Inadequate, these data values are not applicable for the melamine cyanurate complex.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**The melamine cyanurate complex is expected to have limited bioavailability for dermal and inhalation routes of exposure due to its low water solubility under neutral conditions. It is expected to not be absorbed through skin and have poor absorption through the lung and gastrointestinal tract. The dissolution of melamine cyanurate and the solubility and precipitation of melamine and cyanuric acid appear to be pH dependent indicating that ingestion of this compound may enhance bioavailability. Melamine is distributed to the stomach, small intestine, cecum, and large intestine, and found in blood and urine of rats. Cyanuric acid distributes rapidly following oral administration with the highest concentrations found in blood, liver and kidney. The elimination phase half-life for melamine is approximately 3 hours. Cyanuric acid is quickly excreted primarily in the urine as the unchanged compound.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	**Melamine cyanurate**: Not absorbed through skin; poor absorption through lung and gastrointestinal tract (Estimated)	Professional judgment.	Estimated based on limited bioavailability and not expected to be readily absorbed; however, ingested melamine cyanurate could be dissociated to form melamine and cyanuric acid in the low pH environment found in the stomach.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine and cyanuric acid co-exposure: The solubility of melamine and cyanuric acid in urine was higher than in water suggesting a pH dependent effect. The lowest solubility was at a pH of 5–5.5; Solubility in human urine was in the range of 250 mg/L at pH 3 and 8. The solubility limits for melamine and cyanurate increased with increasing pH over the range of 5-8.3 and solubility at pH 5 was 30 mg/L in rats. There is a pH dependent precipitation of melamine and cyanuric acid in rat and human urine. No difference in crystal formation was observed at the 1- or 24-hour time point.	ECHA, 2011a	Study details reported in a secondary source.
		Melamine and cyanuric acid co-exposure: Melamine and cyanuric acid orally (gavage) administered separately formed crystals of melamine cyanurate in the kidneys of rats. There was decreased creatinine clearance, increased in serum creatinine and Blood Urea Nitrogen (BUN) ratio; increased absolute and relative kidney weight.	ECHA, 2011a	Sufficient details reported in a secondary source.
		Melamine: The elimination phase half-life calculated from plasma data was 2.7 hours, and the urinary half-life was 3.0 hours. The renal clearance was determined to be 2.5 mL/min.	Mast et al., 1983	For melamine; adequate, non-guideline study.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Distributed to stomach, small intestine, cecum, and large intestine, and found in blood and urine of rats.	ECHA, 2011b	Study details reported in a secondary source.
		Cyanuric acid: There was 98% recovery of ingested cyanuric acid in urine of 2 volunteers; elimination half-life estimated to be 2.2–3.5 hours; consistent with the one-compartment open model with first order input and elimination; cyanuric acid is excreted rapidly and nearly completely after ingestion.	OECD SIDS, 1999b	Study details reported in a secondary source.
		Cyanuric acid: Distributes rapidly following oral administration to rats; highest concentrations found in blood, liver and kidney with maximum concentrations 30 minutes after dosing; excreted primarily in urine as unchanged substance; poor dermal absorption.	ECHA, 2011b	Sufficient details reported in a secondary source; test substance identified as 2,4,6-isocyanuric acid.
Acute Mammalian Toxicity		**LOW: Estimated based on measured acute oral, dermal, and inhalation toxicity values for the dissolution products melamine and cyanuric acid. The melamine cyanurate complex is also estimated to have limited bioavailability and water solubility that is consistent with a low concern for dermal and inhalation routes of exposure.**		
Acute Lethality	**Oral**	**Melamine:** Rat LD_{50} = 3,161 mg/kg b.w. (male), 3,828 mg/kg (female)	NTP, 1983; Melnick et al., 1984	Sufficient study details reported.
		Melamine: Mouse LD_{50} = 3,296 mg/kg (male), 7,014 mg/kg (female)	NTP, 1983; Melnick et al., 1984	Sufficient study details reported.
		Melamine: Mouse LD_{50} = 4,550 mg/kg	American Cyanamid Company, 1955; May, 1979; Trochimowicz et al., 2001	Sufficient study details were not available. Reported in secondary sources.
		Melamine: Rat LD_{50} = 3,160 mg/kg (male), 3,850 mg/kg (female)	Trochimowicz et al., 2001	Sufficient study details were not reported.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Rat LD_{50} >6,400 mg/kg	BASF, 1969	Sufficient study details were not available.
		Melamine: LD_{50} ≈ 4,800 mg/kg	Hoechst, 1963	Sufficient study details were not available.
		Cyanuric acid: Rat LD_{50} >5,000 mg/kg	ECHA, 2011b	Sufficient study details reported in a secondary source; OECD guideline 420.
		Cyanuric acid: Rat LD_{50} = 7,700 mg/kg	OECD SIDS, 1999b	Reported in a secondary source with limited study details provided; purity unknown.
		Cyanuric acid: Mouse LD_{50} = 3,400 mg/kg	OECD SIDS, 1999b	Reported in a secondary source with limited study details provided; purity unknown.
		Cyanuric acid: Rabbit LD_{50} >10 mg/kg	OECD SIDS, 1999b	Reported in a secondary source with limited study details provided; purity unknown.
	Dermal	**Melamine cyanurate:** Estimated to have limited bioavailability and therefore is of low potential for the dermal route of exposure.	Professional judgment	Based on physical chemical properties including limited bioavailability and low water solubility.
		Melamine: Rabbit LD_{50} >1,000 mg/kg	Unknown, 1990	Sufficient study details were not available.
		Cyanuric acid: Rabbit LD_{50} >7,940 mg/kg	OECD SIDS, 1999b	Reported in a secondary source with limited study details provided; purity unknown.
		Cyanuric acid: Rabbit LD_{50} >5,000 mg/kg	ECHA, 2011b	Sufficient study details reported in a secondary source; OECD guideline 402.
	Inhalation	**Melamine cyanurate:** Estimated to have limited bioavailability and therefore is of low potential for the inhalation route of exposure.	Professional judgment	Based on physical chemical properties including limited bioavailability and low water solubility.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Rat LC_{50} = 3.248 mg/L	Ubaidullajev 1993	The study details, if present, were not translated into English.
		Cyanuric acid: Rat LC_{50} >5.25 mg/L	ECHA, 2011b	Sufficient study details reported in a secondary source; OECD guideline 403.
Carcinogenicity		**MODERATE: Estimated based on the dissolution product melamine. There is evidence that oral melamine exposure causes carcinogenicity in experimental animals; however, there was no evidence located as to its carcinogenicity to humans. Tumor formation in animals appears to happen in a mechanical nature under conditions in which it produces bladder calculi. Cyanuric acid is not carcinogenic. There were no data located as to the carcinogenic potential of the melamine cyanurate complex. IARC classifies melamine as Group 3: *not classifiable as to its carcinogenicity to humans.***		
	OncoLogic Results	**Melamine:** Marginal (Estimated)	OncoLogic, 2005	
	Carcinogenicity (Rat and Mouse)	**Melamine:** Group 3: melamine is not classifiable as to its carcinogenicity to humans; there is inadequate evidence in humans for the carcinogenicity of melamine, and there is sufficient evidence in experimental animals for the carcinogenicity of melamine under conditions in which it produces bladder calculi.	IARC, 1999	IARC classification statement.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Significant formation of transitional cell carcinomas in the urinary bladder of dosed male rats and significant chronic inflammation in the kidney of dosed female rats were observed following exposure in the feed for up to 103 weeks. Carcinoma formation was significantly correlated with the incidence of bladder stones. A transitional-cell papilloma was observed in the urinary bladder of a single high dose male rat, and compound related lesions were observed in the urinary tract of dosed animals. Based on the mechanical nature of tumor formation, FDA and EPA considered melamine noncarcinogenic.	NTP, 1983; Huff, 1984; Melnick et al., 1984	Sufficient study details reported.
		Melamine: Increased incidence of acute and chronic inflammation and epithelial hyperplasia of the urinary bladder was observed in male mice following oral (feed) exposure for up to 103 weeks. Bladder stones and compound related lesions were observed in the urinary tract of test animals. There was no evidence of bladder tumor development. Melamine was not considered carcinogenic.	NTP, 1983; Huff, 1984; Melnick et al., 1984	Sufficient study details reported.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Melamine-induced proliferative lesions of the rat urinary tract were directly due to the irritant stimulation of calculi, and not to molecular interactions between melamine or its metabolites with the bladder epithelium.	Okumura et al., 1992	Sufficient study details reported.
		Melamine: Water intake, used as an index of urinary output, was increased by NaCl treatment. Calculus formation resulting from melamine administration was suppressed dose-dependently by the simultaneous NaCl treatment. The main constituents of calculi were melamine and uric acid (total contents 61.1–81.2%). The results indicate that melamine-induced proliferative lesions of the urinary tract of rats were directly due to the irritation induced-stimulation of calculi, and not molecular interactions between melamine itself or its metabolites with the bladder epithelium.	Ogasawara et al., 1995	Sufficient study details reported.
		Melamine: As an initiator, melamine caused no significant increase in papillomas per mouse when compared to controls.	Perrella and Boutwell, 1983	Sufficient study details reported; non-guideline study.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Diffuse papillary hyperplasia of the bladder epithelium and bladder calculi were observed in all melamine treated rats. Elevated spermidine/spermine N1-acetyltransferase (SAT) activity following melamine treatment was considered to be an indicator of cell proliferation.	Matsui-Yuasa et al., 1992	Sufficient study details reported; non-guideline study.
		Melamine: Decreased antitumor activity was correlated with increasing demethylation; melamine was considered inactive as an antitumor drug.	Rutty and Connors, 1977	Sufficient study details were not available.
		Melamine: In an *in vitro* cytotoxicity study in cultured ADJ/PC6 plasmacytoma ascites tumor cells the ID_{50} was 470 µg/mL after 72 hours of treatment.	Rutty and Abel, 1980	Sufficient study details were not available.
	Combined Chronic Toxicity/ Carcinogenicity	**Melamine:** No effects were observed in rats fed 1,000 ppm of melamine. Four of the 10 rats fed 10,000 ppm of melamine had bladder stones associated with the development of benign papillomas.	Anonymous, 1958	Sufficient study details were not available.
		Melamine: Increased incidence of urinary bladder stones (6/20 rats) was noted in the 10,000 ppm dose group, and was associated with an increase in benign papillomata. The NOAEL was determined to be 1,000 ppm (67 mg/kg).	American Cyanamid Company, 1955	Sufficient study details were not available.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Cyanuric acid: Rat, oral (drinking water), 2-year toxicity and oncogenicity study; there was no evidence of treatment-related carcinogenic effects in tissues or organs in any treatment group.	ECHA, 2011b	Sufficient study details reported in a secondary source; EU Method B.33 (combined chronic toxicity/carcinogenicity test); test substance identified as s-trazinetriol, monosodium salt (monosodium cyanurate monohydrate) 99.7% (equivalent to 77.4% cyanuric acid).
		Cyanuric acid: Mouse, oral (drinking water), 2-year toxicity and oncogenicity study; there was no evidence of treatment-related carcinogenic effects in tissues or organs in any treatment group.	ECHA, 2011b	Sufficient study details reported in a secondary source; EU Method B.33 (combined chronic toxicity/carcinogenicity test); test substance identified as monosodium cyanurate monohydrate (equivalent to 77.5% cyanuric acid).
Genotoxicity		**MODERATE: Estimated based on positive results for chromosomal aberrations *in vivo* in mice exposed to the dissolution product melamine. There were also positive results *in vitro* for DNA synthesis-inhibition in Hela S3 cell and genetic toxicity in *Escherichia coli* WP2s in a microscreen assay following melamine exposure. Cyanuric acid does not cause gene mutations or chromosomal aberrations *in vitro*. There were no data located for melamine cyanurate regarding the genotoxicity endpoint.**		
	Gene Mutation *in vitro*	**Melamine:** Bacterial forward mutation assay: Negative with and without liver activation	Haworth et al., 1983; NCI/NTP, 2007	Sufficient study details reported.
		Melamine: Bacterial forward mutation assay: Negative	Seiler, 1973	Sufficient study details were not available.
		Melamine: Bacterial reverse mutation assay: Negative with and without liver activation	Lusby et al., 1979	Sufficient study details were not available.
		Melamine: Bacterial reverse mutation assay: Negative with and without unspecified metabolic activation	Mast et al., 1982a	Sufficient study details were not available.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: *In vitro* mouse lymphoma test: Negative with and without liver activation	McGregor et al., 1988; NCI/NTP, 2007	Sufficient study details reported.
		Melamine: CHO/HGPRT forward mutation assay: Negative with and without liver activation	Mast et al., 1982a	Sufficient study details were not available.
		Cyanuric acid: Negative for mutagenicity to *S. typhimurium* TA1535, TA1537, TA98, TA100 with and without metabolic activation	OECD SIDS, 1999b	Reported in a secondary source with limited study details provided; purity unknown.
		Cyanuric acid: Negative for bacteriophage Lambda induction in *E. coli* with and without metabolic activation	OECD SIDS, 1999b	Reported in a secondary source with limited study details provided; purity unknown.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	**Melamine cyanurate:** *In vitro* chromosomal aberrations test: Negative in Chinese hamster lung fibroblasts (V79) with and without metabolic activation	ECHA, 2011a	OECD guideline 473.
		Melamine: *In vitro* chromosomal aberrations test: Negative in CHO with and without liver activation	Galloway et al., 1987; NCI/NTP, 2007	Sufficient study details reported.
		Melamine: *In vitro* sister chromatid exchange assay: Negative in CHO with and without liver activation	Galloway et al., 1987; NCI/NTP, 2007	Sufficient study details reported.
		Melamine: *In vitro* sister chromatid exchange assay: Negative in CHO with and without liver activation	Mast et al., 1982a	Sufficient study details were not available.
		Cyanuric acid: Negative for chromosomal aberrations in Chinese hamster lung cells with and without metabolic activation	OECD SIDS, 1999b	Reported in a secondary source with limited study details provided; 99.5% purity.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Cyanuric acid: Negative for sister chromatid exchange in CHO cells with and without metabolic activation	OECD SIDS, 1999b; ECHA, 2011b	Sufficient study details reported in secondary sources; purity equivalent to 77% cyanurate.
	Chromosomal Aberrations *in vivo*	**Melamine:** *In vivo* mouse micronucleus test: The initial test gave a positive trend (P = 0.003) for chromosomal damage; however, both peripheral blood smears and the repeat bone marrow test were negative. The overall conclusion was that melamine does not induce chromosomal damage.	NTP, 1983; Shelby et al., 1993	Sufficient study details reported.
		Melamine: *In vivo* mouse micronucleus test: Negative without activation	Mast et al., 1982b	Sufficient study details were not available.
		Melamine: *In vivo* chromosome aberrations test in mice: Positive	NCI/NTP, 2007	Sufficient study details reported.
		Melamine: *In vivo* sister chromatid exchange assay in mice: Positive	NCI/NTP, 2007	Sufficient study details reported.
	DNA Damage and Repair	**Melamine:** *In vivo* and *in vitro* unscheduled DNA synthesis (UDS) test: None of the tested chemicals, including melamine, were genotoxic hepatocarcinogens in the *in vivo* assay, and melamine was negative for UDS in the *in vitro* assay	Mirsalis et al., 1983	Sufficient study details were not available.
		Melamine: SOS/*umu* test: Negative for its ability to result in DNA damage and induce the expression of the *umu* operon	Reifferscheid and Heil, 1996	Non-guideline study.
		Melamine: DNA synthesis-inhibition test in Hela S3 cells: Inhibits DNA synthesis by 50% (DI_{50}) at >300 µM	Heil and Reifferscheid, 1992	Sufficient study details were not available.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Other	**Melamine:** Sex-linked recessive lethal/reciprocal translocation: Results were considered equivocal based on 0.18% and 0.36% total lethal following oral and injection exposure, respectively, compared to control total lethal of 0.07% for oral and 0.09% for injection	NCI/NTP, 2007	Sufficient study details reported.
		Melamine: Drosophila Muller-5 test: Negative for mutagenicity	Rohrborn, 1959	Sufficient study details were not available.
		Melamine: *Drosophila melanogaster* Sex-linked recessive lethal: No mutagenic effects were observed.	Luers and Rohrborn, 1963	Sufficient study details were not available.
		Melamine: *In vitro* flow cytometric DNA repair assay: Negative for genotoxic effects	Seldon et al., 1994	Non-guideline study.
		Melamine: Microscreen assay: Positive for genetic toxicity in *E.coli* WP2s	Rossman et al., 1991	Non-guideline study.
		Melamine: Growth and genotoxic effects to bacteria (*Salmonella typhimurium)* and yeast *(Saccharomyces cerevisiae):* Non-mutagenic in *S.typhimurium* with or without S-9 mix. The growth of eight out of nine strains tested was delayed by 10 mM melamine during 24-hour cultivation. *S.cerevisiae* strain was tested, and did not recover its growth following 48-hour cultivation.	Ishiwata et al., 1991	Sufficient study details were not available.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Reproductive Effects		**MODERATE: Potential for reproductive toxicity estimated based on data for a confidential analog that reports a NOAEL of 1,600 ppm (191-341 mg/kg/day) in rats orally exposed. Data based on the dissolution products indicate no effects on reproductive parameters in rats orally exposed to cyanuric acid for up to 3 generations or when exposed to melamine in a 13-week toxicity study. There were no data located regarding reproductive toxicity following exposure to melamine cyanurate.**		
	Reproduction/ Developmental Toxicity Screen	Rat, oral; potential for reproductive toxicity NOAEL = 1,600 ppm (191-341 mg/kg/day) (Estimated by analogy)	Professional judgment	Estimated based on analogy to confidential analog; LOAEL not identified; study details not provided.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	**Cyanuric acid:** Rat, oral (gavage), males exposed for 45 days, females exposed from 14 days prior to mating to LD 3; there were no effects on reproductive parameters including copulation index, fertility index, gestation length, numbers of corpora lutea or implantations, implantation index, gestation index, delivery index and behavior at delivery and lactation. NOAEL ≥600 mg/kg/day (highest dose tested)	OECD SIDS, 1999b	Reported in a secondary source; conducted according to OECD guidelines; 99.8% purity. LOAEL not established for reproductive toxicity.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Cyanuric acid: Rat, oral, exposure initiated at 36 days of age to F_0 generation, 21 days to F_1 and F_2 parents and administered until termination of each generation; F_0 males and females exposed minimum of 100 days, F_1 and F_2 male and females exposed a minimum of 120 days; There were no treatment-related reproductive effects observed. NOAEL $F_0 \geq \sim 470$ mg/kg-day (male) NOAEL $F_0 \geq \sim 950$ mg/kg-day (female)	ECHA, 2011b	Sufficient study details reported in secondary source; EU Method B.35 (two-generation reproduction toxicity test); test substance identified as sodium salt of cyanuric acid (equivalent to 77.5% cyanuric acid.
	Reproduction and Fertility Effects	**Melamine:** There were no treatment-related macroscopic or microscopic effects on mammary glands, ovaries, prostate, seminal vesicles, testes and uterus in rats and mice in a 13-week study.	OECD, 1999a	Study details, including administered dose information, were not provided.
Developmental Effects		**MODERATE: Estimated based on analogy to nitrogen heterocycles. Data for dissolution products melamine and cyanuric acid indicate no developmental effects in rats orally exposed to cyanuric acid or melamine during gestation. There were no data located regarding developmental toxicity following exposure to melamine cyanurate.**		
	Reproduction/ Developmental Toxicity Screen	Potential for developmental toxicity (Estimated by analogy)	Professional judgment	Estimated based on analogy to nitrogen heterocycles.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	**Cyanuric acid:** Rat, oral (gavage), males exposed for 45 days, females exposed from 14 days prior to mating to LD 3. There were no effects in offspring parameters including number sex ratio, live birth and viability indices, body weight, or incidences of external and visceral abnormalities. NOAEL ≥600 mg/kg/day (highest dose tested)	OECD SIDS, 1999b	Reported in a secondary source; conducted according to OECD guidelines; 99.8% purity. LOAEL not established for developmental toxicity.
		Cyanuric acid: Rat, oral, exposure initiated at 36 days of age to F_0 generation, 21 days to F_1 and F_2 parents and administered until termination of each generation; F_0 males and females exposed minimum of 100 days, F_1 and F_2 male and females exposed a minimum of 120 days. There were no treatment-related developmental effects observed. NOAEL $F_0 \geq \sim 470$ mg/kg-day (male) NOAEL $F_0 \geq \sim 950$ mg/kg-day (female)	ECHA, 2011b	Sufficient study details reported in secondary source; EU Method B.35 (two-generation reproduction toxicity test); test substance identified as sodium salt of cyanuric acid (equivalent to 77.5% cyanuric acid).
	Prenatal Development	**Melamine:** Signs of maternal toxicity at 136 mg/kg-day included decreased body weight and feed consumption, hematuria (23/25 rats), indrawn flanks (7/25 rats), and piloerection (1/25 rats). No adverse effects on gestational parameters and no signs of developmental toxicity were noted. NOAEL ≥1,060 mg/kg-day	Hellwig et al., 1996	Study details reported in a secondary source.

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Cyanuric acid: Rat, oral (gavage); exposure on GD 6-15; There were no developmental effects observed. NOAEL = 5,000 mg/kg-day (highest dose tested)	ECHA, 2011b	Sufficient study details reported in a secondary source; EU method B.31 (prenatal developmental toxicity study); test substance identified as monosodium cyanurate monohydrate; 99% purity (equivalent to 77.4% cyanuric acid).
	Postnatal Development			No data located.
Neurotoxicity		**LOW: Estimated to not have potential for neurotoxicity based on expert judgment.**		
	Neurotoxicity Screening Battery (Adult)	Potential for neurotoxicity is expected to be low (Estimated)	Expert judgment	Estimated based on expert judgment.
Repeated Dose Effects		**HIGH: Based on kidney toxicity following repeated oral exposure to melamine cyanurate and simultaneous co-exposure to melamine and cyanuric acid in rats. Kidney effects included increased plasma BUN and creatinine levels, the formation of precipitates in the kidney and acute renal failure. Repeated oral exposure to the dissolution product melamine also results in urinary bladder stones at doses in the moderate hazard range. The hazard designation for cyanuric acid is considered to be low.**		
		Melamine cyanurate: Rat, 7-day feeding study. Increased plasma BUN and creatinine levels at 666 ppm (66.6 mg/kg/day (nominal); severe kidney toxicity at 2,000 ppm (200 mg/kg-day); formation of precipitates in the kidney. There were also mortality, signs of toxicity, decreased body weight and food consumption, changes in organ weights, gross pathology and non-neoplastic histopathology at higher doses. NOEL: 200 ppm (~ 10 mg/kg-day) LOAEL: 660 ppm (`~ 66.6 mg/kg-day) – based on increased plasma BUN and creatinine levels.	ECHA, 2011a	Reported in a secondary source. Study designed to test kidney toxicity; test substance identified as melaminzyanurat; purity > 99%.

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine and cyanuric acid co-exposure: Rat, oral 14-day oral (gavage) study of melamine and cyanuric acid co-exposure (each at 1.2, 12, 120 mg/kg-day); crystal formation in renal distal tubular lumens and collecting ducts were observed on day 3 in the 12 mg/kg-day group; crystal in proximal tubular lumens of renal cortex on day 3 and mortal acute renal failure on day 7 occurred at doses of 120 mg/kg-day. NOEL: 1.2 mg/kg-day LOEL: 12 mg/kg-day (based on crystals of melamine cyanurate in kidneys)	ECHA, 2011a	Reported in a secondary source. Study focused on renal crystal formation.
	Melamine and cyanuric acid co-exposure: 7-day feeding study in rats; Signs of toxicity evident, at doses of 33 mg/kg-day, there were pale yellow and enlarged kidneys and increased BUN and serum creatinine; histopathological evaluation showed golden brown crystals in renal tubules of all rats at this dose. There were no significant differences in kidney weights or crystals tor tubular changes in rats administered melamine (200 mg/kg-day) or cyanuric acid (200 mg/kg-day) alone. NOAEL: 10 mg/kg-day LOAEL: 33 mg/kg-day (based on kidney toxicity)	ECHA, 2011a; Jacob et al. 2011	Both melamine and cyanurate were added to feed with a 1:1 ratio; primary source.

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine and cyanuric acid co-exposure: Melamine and cyanuric acid orally (gavage) administered separately formed crystals of melamine cyanurate in kidney of rats. There was decreased creatinine clearance, increased in serum creatinine and BUN; increased absolute and relative kidney weight	ECHA, 2011a	Reported in a secondary sources. Effect levels not identified.
	Melamine: Rat 28-day dietary toxicity study: Clinical signs included a dose-related increase in pilo-erection, lethargy, bloody urine spots in the cage and on the pelage of animals, and chromodacryorrhea. The incidence of urinary bladder calculi and urinary bladder hyperplasia in treated animals was dose dependent, with a significant relationship between the calculi and hyperplasia. Calculi composition indicated the presence of an organic matrix containing melamine, phosphorus, sulfur, potassium, and chloride. Crystals of dimelamine monophosphate were identified in the urine. NOAEL: 2,000 ppm (240 mg/kg/day), excluding the observed increase in water consumption and the incidence of crystalluria. LOAEL: 4,000 ppm (475 mg/kg/day) based on the formation of calculi.	RTI, 1983	Sufficient study details reported.

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine: Rabbit and dog 28-day dietary toxicity study: No significant rise in the body temperature of rabbits was noted. Gross histological examination of the heart, lung, liver, spleen, thyroid, pancreas, intestines, kidneys and bladder did not show pathological changes. A zone of fat was found in the inner part of the renal cortex in two dogs, but also in the kidneys of 3 control dogs.	Lipschitz and Stokey, 1945	Sufficient study details were not available.
	Melamine: Rat 28-day dietary toxicity study: Incidence and size of bladder stones were directly related to the amount of substance administered. The larger stones were found to be unchanged melamine in a matrix of protein, uric acid and phosphate. Lowest effect dose (LED): 1,500 ppm (~125 mg/kg) in males.	American Cyanamid Company, 1984	Sufficient study details were not available.

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine: Rat 90-day dietary toxicity study: One male rat receiving 18,000 ppm and two males receiving 6,000 ppm died. Mean body weight gain and feed consumption were reduced. Stones and diffuse epithelial hyperplasia in the urinary bladders were observed in male rats of all treatment groups. Focal epithelial hyperplasia was observed in only 1 male. A second and third 13-week repeated dose toxicity study was conducted in rats at a dose range of 750 to 18,000 ppm; bladder stones were observed at all dose levels. At 18,000 ppm, stones occurred in diets with and without the addition of ammonium chloride to drinking water. LOAEL = 700 ppm (72 mg/kg/day)	NTP, 1983; Melnick et al., 1984; ECHA, 2011a	Sufficient study details reported.

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine: Mouse 90-day dietary toxicity study: a single female mouse died after receiving 9,000 ppm. Mean body weight gain relative to controls was depressed. The incidence of mice with bladder stones was dose-related and was greater in males than in females. Sixty percent of mice having bladder ulcers also had urinary bladder stones. Bladder ulcers were multifocal or associated with inflammation (cystitis). Epithelial hyperplasia and bladder stones were observed together in 2 mice. Also, epithelial cell atypia was seen. NOAEL: 6,000 ppm (600 mg/kg-day). LOAEL: 9,000 ppm (900 mg/kg-day)	NTP, 1983; Melnick et al., 1984	Sufficient study details reported.
	Melamine: Increased incidence of acute and chronic inflammation and epithelial hyperplasia of the urinary bladder was observed in mice following oral (feed) exposure for up to 103 weeks. There was also increased incidence of bladder stones in male mice. LOAEL = 2,250 mg/kg diet (lowest dose tested)	NTP, 1983; ECHA, 2011a	Repeated dose effects described in a carcinogenicity bioassay study.
	Melamine: Dog 1-year dietary toxicity study: crystalluria started 60 to 90 days into treatment, and persisted during the study period. No other effects attributable to melamine were observed.	American Cyanamid Company, 1955	Sufficient study details were not available.

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PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine: Rat 30-month dietary toxicity study: Neither accumulation of calculi nor any treatment-related urinary bladder lesions were found.	Mast et al., 1982c	Sufficient study details were not available.
	Melamine: Rat 24- to 30-month dietary toxicity study: A dose related trend for dilated glands in glandular gastric mucosa and inflammation in non glandular gastric mucosa was observed. Urinary bladder calculi formation was not observed.	American Cyanamid Company, 1983	Sufficient study details were not available.

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Cyanuric acid: Rat, oral (gavage), combined repeat dose and reproductive/developmental toxicity screening test; males exposed for 44 days, females exposed from 14 days prior to mating to LD day 3. Toxic effects included: reddish urine, decreased body weight gain (males), increased erythrocytes and leukocytes in urine, decreased erythrocyte count, hemoglobin, and heatocrit (male), increased urea nitrogen and creatinine, decreased sodium (male), dilation of renal tubules, necrosis or hyperplasia of the tubular epithelium, increased basophilic tubules, neutrophilic infiltration, mineralization and fibrosis in the kids, hyperplasia of the mucosal epithelium in urinary bladder and vacuolization of the zona fasciculate in the adrenals, increased absolute and relative kidney weight and relative adrenal weights (both sexes), atrophic thymus (females). NOAEL = 150 mg/kg/day LOAEL = 600 mg/kg/day	OECD SIDS, 1999b	Reported in a secondary source with limited study details provided; 99.8% purity.

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Cyanuric acid: Rat, oral (drinking water), 2-year toxicity and oncogenicity study; red urine in males at the highest dose was observed (371 mg/kg-day); there were no treatment-related changes in hematology, clinical chemistry, urinalysis, or organ weights; non-neoplastic lesion in urinary tracts and heart and urinary tract lesions of males exposed to 5,375 ppm (371 mg/kg-day) for 6-12 months; There were no treatment-related lesions in rats exposed for 18 or 24 months. NOAEL = 154 mg/kg-day (male) LOAEL = 371 mg/kg-day (male)	ECHA, 2011b	Sufficient study details reported in a secondary source; EU Method B.33 (combined chronic toxicity/carcinogenicity test); test substance identified as s-trazinetriol, monosodium salt (monosodium cyanurate monohydrate) 99.7% (equivalent to 77.4% cyanuric acid).
	Cyanuric acid: Mouse, oral (drinking water), 2-year toxicity and oncogenicity study; there were no treatment-related effects. NOAEL ≥ 1,520 mg/kg-day (male) NOAEL ≥ 1,580 mg/kg-day (female)	ECHA, 2011b	Sufficient study details reported in a secondary source; EU Method B.33 (combined chronic toxicity/carcinogenicity test); test substance identified as monosodium cyanurate monohydrate (equivalent to 77.5% cyanuric acid).
	Cyanuric acid: Mouse, oral (drinking water), 13-week subchronic toxicity study; there were no treatment related effects at doses as high as 1,523 mg/kg-day (males) and 1,582 mg/kg-day (females) NOAEL ≥1,523 mg/kg-day (male) NOAEL ≥1,582 mg/kg-day (female)	ECHA, 2011b	Sufficient study details reported in a secondary source; test substance identified as s-trazinetriol, monosodium salt (monosodium cyanurate monohydrate) 99.5% (equivalent to 76.9% cyanuric acid).

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Cyanuric acid: Rat, oral (drinking water, 13-week toxicity study; there were no treatment-related effects NOAEL ≥521 mg/kg-day (male) NOAEL ≥717 mg/kg-day (female)	ECHA, 2011b	Sufficient study details reported in a secondary source; test substance identified as s-trazinetriol, monosodium salt (monosodium cyanurate monohydrate) (equivalent to 77.34% cyanuric acid.
Skin Sensitization		**LOW: Estimated based on evidence of mild skin sensitization following exposure to the dissolution product cyanuric acid. Melamine, also a dissolution product of melamine cyanurate, was not a skin sensitizer to humans or guinea pigs. There was no data located for melamine cyanurate for skin sensitization.**		
	Skin Sensitization	**Melamine:** No evidence of primary dermal irritation or sensitization in a human patch test	American Cyanamid Company, 1955; Trochimowicz et al., 2001	Sufficient study details were not available.
		Melamine: Non-sensitizing to guinea pigs	Fasset et al.,1963/1981; Trochimowicz et al., 2001	Sufficient study details were not available.
		Cyanuric acid: Borderline or mild skin sensitization in mice.	ECHA, 2011b	Sufficient study details reported in a secondary source; OECD guideline 429.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Estimated based on mild-to-moderate irritation to rabbit eyes following exposure to the dissolution products melamine and cyanuric acid. There was no data located for melamine cyanurate for eye irritation.**		
	Eye Irritation	**Melamine:** Non-irritating to rabbit eyes	BASF, 1969	Sufficient study details were not available.
		Melamine: Non-irritating to rabbit eyes following 0.5 mL of 10% melamine	American Cyanamid Company, 1955; Trochimowicz et al., 2001	Sufficient study details were not available.
		Melamine: Mild irritant to rabbit eyes following exposure to 30 mg of dry powder	American Cyanamid Company, 1955; Trochimowicz et al., 2001	Sufficient study details were not available.
		Melamine: Slightly irritating to rabbit eyes	Marhold, 1972	Sufficient study details were not available.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Cyanuric acid: Slightly to moderately irritating to rabbit eyes	OECD SIDS, 1999b	Sufficient study details reported in secondary source; OECD guideline 405.
		Cyanuric acid: Slightly irritating to rabbit eyes	ECHA, 2011b	Sufficient study details reported in a secondary source; OECD guideline 405; fully reversible within: 3 days.
Dermal Irritation		**LOW: Estimated based on slight irritation to rabbit skin following exposure to the dissolution product cyanuric acid. Melamine, also a dissolution product of melamine cyanurate was not irritating to rabbit skin. There were no data located for melamine cyanurate for skin irritation.**		
	Dermal Irritation	**Melamine:** Not irritating to rabbit skin	Rijcken, 1995	OECD 404 guideline study.
		Melamine: Not irritating to rabbit skin	BASF, 1969	Sufficient study details were not available.
		Melamine: Not irritating to rabbit skin	American Cyanamid Company, 1955; Trochimowicz et al., 2001	Sufficient study details were not available.
		Melamine: Not irritating to rabbit skin	Fasset et al., 1963/1981; Trochimowicz et al., 2001;	Sufficient study details were not available.
		Cyanuric acid: Slightly irritating to rabbit skin	OECD SIDS, 1999b, ECHA, 2011b	Sufficient study details reported in a secondary source; OECD guideline 404.
Endocrine Activity		**There were insufficient data located to describe the effect of melamine cyanurate on the endocrine system. In one study, melamine did not exhibit estrogenic activity *in vitro* in a yeast two-hybrid assay.**		
		Melamine: Showed no estrogenic activity (no change in B-galactosidase activity) in an *in vitro* yeast two-hybrid assay in *Saccharomyces cerevisia* Y 190	ECHA, 2011a	Reported in a secondary source. Non-guideline study.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Immunotoxicity		**Located data were not sufficient to determine the hazard potential for this endpoint.**		
	Immune System Effects	**Melamine:** Did not inhibit the mitogenesis of B- and T- lymphocytes in an *in vitro* mouse lymphocyte mitogenesis test.	ECHA, 2011a	Reported in a secondary source. Unclear how well mitogenesis test assesses immunotoxicity of chemicals.
ECOTOXICITY				
ECOSAR Class		Melamine: Anilines (amino-meta), Melamines; Cyanuric acid: Aromatic triazines		
Acute Toxicity		**LOW: Melamine cyanurate has low water solubility and therefore it is estimated that it will display no effects at saturation (NES) because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. A low hazard concern is also assigned for the dissociation products, melamine and cyanuric acid, based on experimental data.**		
Fish LC_{50}		**Melamine cyanurate**:	No data located.	Not amenable to estimation by available models that cannot accept chemicals with complex organic cations and anions.
		Melamine cyanurate: Melamine cyanurate has low water solubility and therefore it is estimated that it will display NES.	Professional judgment	The amount of melamine cyanurate dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.
		Melamine *: Leuciscus idus melanotus* 48-hour LC_{50} >500 mg/L (Experimental)	OECD SIDS, 1999a	Study details reported in a secondary source.
		Melamine: *Oryzias latipes* 48-hour LC_{50} = 1,000 mg/L (Experimental)	OECD SIDS, 1999a	Study details reported in a secondary source.
		Melamine: *Poecilia reticulata* 96-hour LC_{50} >3,000 mg/L (Experimental)	OECD SIDS, 1999a	Study details reported in a secondary source.
		Melamine: *Poecilia reticulata* 4,400 mg/L dose lethal to <10% (Experimental)	OECD SIDS, 1999a	Study details reported in a secondary source.

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PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine: Fish 96-hour LC_{50} = 2,680 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	EPI	
	Melamine: Fish 96-hour LC_{50} = 391 mg/L (Estimated) ECOSAR: Melamines	EPI	
	Melamine: Fish 96-hour LC_{50} = 14,272 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Cyanuric acid: *Oryzias latipes* 96-hour LC_{50} >100 mg/L Semi-static and flow-through open conditions (Experimental)	OECD SIDS 1999b	Cyanuric acid (99.7% purity); study details reported in a secondary source; separate experiments conducted with flow-through and semi-static conditions according to OECD TG203 guidelines.
	Cyanuric acid: *Lepomis macrochirus* (fathead minnow) 96-hour LC_{50} >1,000 mg/L Static conditions (Experimental)	ECHA, 2011b	Cyanuric acid; purity unknown; not a guideline study but well reported in a secondary source.
	Cyanuric acid: *Pimephales promelas* (bluegill sunfish) 96-hour LC_{50} >2,100 mg/L Static conditions (Experimental)	ECHA, 2011b	Cyanuric acid; well reported in a secondary source.
	Cyanuric acid: Fish 96-hour LC_{50} = 72.04 mg/L (Estimated) ECOSAR: Aromatic triazines	EPI	

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Cyanuric acid: Fish 96-hour LC_{50} = 116.98 mg/L (Estimated) ECOSAR: Neutral organics	EPI	

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Daphnid LC_{50}	**Melamine cyanurate**:	No data located.	Not amenable to estimation by available models that cannot accept chemicals with complex organic cations and anions.
	Melamine cyanurate: Melamine cyanurate has low water solubility and therefore it is estimated that it will display NES.	Professional judgment	The amount of melamine cyanurate dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.
	Cyanuric acid: *Daphnia magna* 48-hour EC_{50} = 1,000 mg/L (immobilization); static, open-system conditions (Experimental)	OECD SIDS 1999b	Cyanuric acid (99.7% purity); study details reported in a secondary source; study conducted according to OECD TG202 guidelines; 1,000 mg/L was the highest dose tested.
	Cyanuric acid: *Daphnia magna* 48-hour LC_{50} >1,000 mg/L Static conditions (Experimental)	ECHA, 2011b	Cyanuric acid; not a guideline study, but well reported in a secondary source; purity not known.
	Cyanuric acid: Daphnid 48-hour LC_{50} = 34.65 mg/L (Estimated) ECOSAR: Aromatic triazines	EPI	
	Cyanuric acid: Daphnid 48-hour LC_{50} = 61.33 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Melamine: Daphnid 48-hour LC_{50} = 6.23 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	EPI	
	Melamine: Daphnid 48-hour LC_{50} = 144.34 mg/L (Estimated) ECOSAR: Melamines	EPI	

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine: Daphnid 48-hour LC_{50} = 4,805 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
Green Algae EC_{50}	**Melamine cyanurate**:	No data located.	Not amenable to estimation by available models that cannot accept chemicals with complex organic cations and anions.
	Melamine cyanurate: Melamine cyanurate has low water solubility and therefore it is estimated that it will display NES.	Professional judgment	The amount of melamine cyanurate dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.
	Melamine: *Scenedesmus pannonicus* 4-day EC_{50} = 940 mg/L (Experimental); 4-day NOEC = 320 mg/L (Experimental)	OECD SIDS, 1999a	Reported in a secondary source, study details and test conditions were not provided.
	Melamine: Green algae 96-hour EC_{50} = 2.79 mg/L (Estimated) ECOSAR class: Anilines (amino-meta)	EPI	
	Melamine: Green algae 96-hour EC_{50} = 325 mg/L (Estimated) ECOSAR class: Melamines	EPI	
	Melamine: Green algae 96-hour EC_{50} = 4,396 mg/L (Estimated) ECOSAR class: Neutral organics	EPI	
	Cyanuric acid: *Selenastrum capricornutum* 72-hour EC_{50} = 620 mg/L (biomass) 72-hour NOEC = 62.5 mg/L (Experimental)	OECD SIDS, 1999b	Cyanuric acid (99.7% purity); study details reported in a secondary source; study conducted according to OECD TG201 guidelines.

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Cyanuric acid: Green algae 96-hour EC_{50} = 0.11 mg/L (Estimated) ECOSAR: Aromatic triazines	EPI	
	Cyanuric acid: Green algae 96-hour EC_{50} = 56.87 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
Chronic Aquatic Toxicity	**LOW: Melamine cyanurate has low water solubility and therefore it is estimated that it will display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. A low hazard concern is also for assigned for the dissociation products, melamine and cyanuric acid, based on experimental data.**		
Fish ChV	**Melamine cyanurate**:	No data located.	Not amenable to estimation by available models that cannot accept chemicals with complex organic cations and anions.
	Melamine cyanurate: Melamine cyanurate has low water solubility and therefore it is estimated that it will display NES.	Professional judgment	The amount of melamine cyanurate dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.
	Melamine: *Jordanella floridae* 35-day NOEC ≥ 1,000 mg/L (Experimental)	OECD SIDS, 1999a	Reporteded in a secondary source, study details and test conditions were not provided.
	Melamine: *Salmo gairdneri* NOEC (macroscopic) = 500 mg/L (Experimental); NOEC (microscopic) <125 mg/L (Experimental)	OECD SIDS, 1999a	Reported in a secondary source, study details and test conditions were not provided.
	Melamine: *Daphnia magna* 21-day LC_{50} = 32-56 mg/L, 21-day LC_{100} = 56 mg/L, 21-day NOEC = 18 mg/L (Experimental)	OECD SIDS, 1999a	Reported in a secondary source, study details and test conditions were not provided.

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine: Fish ChV = 263 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	EPI	The toxicity value was estimated through application of acute-to-chronic ratios.
	Melamine: Fish ChV = 1,102 mg/L (Estimated) ECOSAR: Melamines	EPI	
	Melamine: Fish ChV = 1,076 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Cyanuric acid: Oncorhynchus mykiss (rainbow trout) 28-day LOEC ≥1,000 mg/L (based on growth rate) Semi-static conditions (Experimental)	ECHA, 2011b	Cyanuric acid; OECD guideline 215; well reported in a secondary source; >97% purity.
	Cyanuric acid: Fish ChV = 1.85 mg/L (Estimated) ECOSAR: Aromatic triazines	EPI	
	Cyanuric acid: Fish ChV = 11.38 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
Daphnid ChV	**Melamine cyanurate**:	No data located.	Not amenable to estimation by available models that cannot accept chemicals with complex organic cations and anions.
	Melamine cyanurate: Melamine cyanurate has low water solubility and therefore it is estimated that it will display NES.	Professional judgment	The amount of melamine cyanurate dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Cyanuric acid: *Daphnia magna* 21-day EC_{50} = 65.9 mg/L (reproduction rate); NOEC = 32.0 mg/L Semi-static, open-system conditions (Experimental)	OECD SIDS 1999b	Cyanuric acid (99.7% purity); study details reported in a secondary source; study conducted according to OECD TG202 guidelines.
	Cyanuric acid: *Daphnia magna* 21-day EC_{50} = 2,117 mg/L cyanuric acid (immobilization) LOEC = 378 mg/L cyanuric acid (mortality and reproduction) NOEC = 121 mg/L cyanuric acid Static conditions (Experimental)	ECHA, 2011b	Cyanuric acid; OECD guideline 211; well reported in a secondary source; >97% purity.
	Cyanuric acid: Daphnid ChV = 1.49 mg/L (Estimated) ECOSAR class: Aromatic triazines	EPI	
	Cyanuric acid: Daphnid ChV = 6.37 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Melamine: Daphnid ChV = 0.078 mg/L (Estimated) ECOSAR class: Anilines (amino-meta)	EPI	
	Melamine: Daphnid ChV = 14.85 mg/L (Estimated) ECOSAR: Melamines	EPI	The toxicity value was estimated through application of acute-to-chronic ratios.
	Melamine: Daphnid ChV = 343.93 mg/L (Estimated) ECOSAR: Neutral organics	EPI	

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Green Algae ChV	**Melamine cyanurate**:	No data located.	Not amenable to estimation by available models that cannot accept chemicals with complex organic cations and anions.
	Melamine cyanurate: Melamine cyanurate has low water solubility and therefore it is estimated that it will display NES.	Professional judgment	The amount of melamine cyanurate dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.
	Melamine: Green algae ChV = 0.70 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	EPI	The toxicity value was estimated through application of acute-to-chronic ratios.
	Melamine: Green algae ChV = 81.26 mg/L (Estimated) ECOSAR: Melamines	EPI	The toxicity value was estimated through application of acute-to-chronic ratios.
	Melamine: Green algae ChV = 313.17 mg/L (Estimated) ECOSAR: Neutral organics	EPI	

Melamine Cyanurate CASRN 37640-57-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Cyanuric acid: *Navicula pelliculosa* 72-hour EC_{50} = 2,041 mg/L cyanuric acid (biomass) 96-hour EC_{50} >3,780 mg/L cyanuric acid (biomass) 72-hour EC_{50} >3,780 mg/L cyanuric acid (growth rate) 96-hour EC_{50} >3,780 mg/L cyanuric acid (growth rate) 72-hour NOEC= 945 mg/L cyanuric acid 96-hour NOEC= 3,780 mg/L cyanuric acid Static conditions (Experimental)	ECHA, 2011b	Cyanuric acid; ISO 10253; well reported in a secondary source; 99.1% purity.
	Cyanuric acid: *Selenastrum capricornutum* 24-hour EC_{50} >1,000 mg/L (based on decreased *in vivo* chlorophyll alpha) 48-hour EC_{50} >1,000 mg/L (based on decreased *in vivo* chlorophyll alpha) 72-hour EC_{50} = 872 mg/L (based on decreased number of cells) 96-hour EC_{50} >712 mg/L (based on decreased number of cells) (Experimental)	ECHA, 2011b	Cyanuric acid; not a guideline study, but test procedures followed those of U.S. EPA Algal Assay Procedure: Bottle test (1971);well reported in a secondary source; 77.5% purity.
	Cyanuric acid: Green algae ChV = 0.06 mg/L (Estimated) ECOSAR: Aromatic triazines	EPI	
	Cyanuric acid: Green algae ChV = 12.55 mg/L (Estimated) ECOSAR: Neutral organics	EPI	

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**The measured low water solubility and estimated low vapor pressure indicate that melamine cyanurate is anticipated to partition predominantly to soil and sediment. Melamine cyanurate is not expected to migrate from soil to groundwater; aromatic amines tend to bind with humic matter in soil. It is not expected to volatilize from water. Volatilization from dry surface is also not expected based on its vapor pressure. In the atmosphere, melamine cyanurate is expected to exist solely in the particulate phase, based on its estimated vapor pressure. Particulates may be removed from air by wet or dry deposition.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment	Cutoff value for non volatile compounds based on the ionic nature of the material.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>1,000 (Estimated)	Professional judgment	Driven by structural analysis of melamine; aromatic amines form covalent bonds to humic matter in soils and sediments, binding irreversibly.
	Level III Fugacity Model			Not all input parameters for this model were available to run the estimation software (EPI) for the hydrogen bonded melamine cyanurate complex.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Persistence		**VERY HIGH: Based on an experimental biodegradation study (OECD 301B) that demonstrated it was not readily biodegradable. This result is consistent with its negligible water solubility suggesting that it is not likely to be readily assimilated by microorganisms. Other degradative processes are not expected to be operative under environmental conditions. Melamine cyanurate is not expected to undergo complete dissolution under neutral conditions, nor under the pHs typically found in the environment. However, it rapidly dissociates under pH extremes. It is least soluble at pH 5 but most soluble at pH 3.5 and below. Melamine cyanurate does not contain chromophores that absorb at wavelengths >290 nm, indicating that it is not expected to be susceptible to direct photolysis by sunlight. The dissociation products, melamine and cyanuric acid salts, have experimental studies indicating that they are not expected to biodegrade under aerobic conditions when assessed as their corresponding neutral organic components. However, experimental studies indicate that cyanuric acid may degrade in anoxic environs.**		
Water	**Aerobic Biodegradation**	**Melamine cyanurate:** Not readily biodegradable according to OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) (Measured)	ECHA, 2011a	Adequate, guideline study.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Soil	**Aerobic Biodegradation**	**Melamine:** Not readily biodegradable: 0% biodegradation detected after 2 weeks with 100 ppm in 30 ppm activated sludge (OECD TG 301C) (Measured); 0% degradation after 28 days with 100 mg DOC/L in activated sludge (Zahn-Wellens test, OECD 302B) (Measured) **Cyanuric Acid:** Not readily biodegradable: 0% biodegradation detected after 2 weeks with 100 ppm in 30 ppm activated sludge (0% BOD; 7.8% TOC) (OECD TG 301C) (Measured)	MITI, 1998; OECD SIDS, 1999a	Adequate values from guideline studies for the melamine cyanurate complex components.
	Anaerobic Biodegradation	**Melamine:** Not probable (Anaerobic-methanogenic biodegradation probability model) **Cyanuric Acid:** 100% degradation after 72-96 hours in anaerobic sewage at 10 µg/mL (Measured); 0% methane production after 1-year incubation in anoxic aquifer slurries (Measured)	Professional judgment; EPI; Saldick. 1974; Adrian and Suflita, 1994	Inadequate, these data values are not applicable for the melamine cyanurate complex.
	Soil Biodegradation w/ Product Identification	**Melamine:** Nitrification of melamine occurs in soil at a low rate (0.7 % organic N found as NO_3-N in week 10, and 0 % in week 28). (Measured) **Cyanuric Acid:** 35 % nitrification at week 10 and 73 % at week 28. (Measured)	ECHA, 2011a	Non-guideline studies for the melamine cyanurate complex components.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	**Melamine:** 16 days (Estimated) **Cyanuric Acid:** 43 hours (Estimated)	EPI	

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine Cyanurate: The test substance was found to be thermally stable within the range 40-290°C according to a method similar to OECD Guideline 113 (Screening Test for Thermal Stability and Stability in Air)	ECHA, 2011a	Non-guideline study.
Reactivity	**Photolysis**	**Melamine Cyanurate, Melamine and Cyanuric acid:** Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	These substances do not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
	Hydrolysis	**Melamine Cyanurate:** The effect of pH on the solubility of melamine cyanurate has established that the minimum lies at pH 5. Decreasing the pH results in the formation of melamine cations and cyanuric acid in solution at pH 3.5 and below. Increasing the pH from 5 to 7.5 results in only a marginal increase in the dissolution of the melamine cyanurate complex. (Measured)	WHO, 2009	These results are consistent with that expected in a closed system. Under environmental conditions, infinite dilution may alter the equilibrium of the process towards enhanced dissolution.
Environmental Half-life		**Melamine Cyanurate:** >1 year (Estimated) **Melamine:** 75 days (Estimated) **Cyanuric Acid:** 30 days (Estimated)	Professional judgment; EPI; PBT Profiler	Melamine cyanurate is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to be removed by other degradative processes under environmental conditions because of its limited water solubility and limited partitioning to air.

Melamine Cyanurate CASRN 37640-57-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Bioaccumulation		**LOW: Melamine cyanurate has negligible water solubility under near neutral conditions and is expected to have poor bioavailability resulting in low potential for bioaccumulation. In addition, experimental BCF data for the organic components of melamine cyanurate, melamine and cyanuric acid are <100. These experimental values also indicate a low potential for bioaccumulation.**		
	Fish BCF	**Melamine Cyanurate:** <100 (Estimated)	Professional judgment	This estimated value is based on the BCF results for the components melamine and cyanurate.
		Melamine: <0.38 in carp (*Cyprinus carpio*) after 6 weeks at 2.0 ppm concentration; <3.8 in carp (*Cyprinus carpio*) after 6 weeks at 0.2 ppm concentration (OECD 302B) (Measured) **Cyanuric Acid:** <0.1 in carp (*Cyprinus carpio*) after 6 weeks at 10 ppm concentration; <0.5 in carp (*Cyprinus carpio*) after 6 weeks at 1 ppm concentration (Measured)	MITI, 1998	Adequate values from guideline studies for the melamine cyanurate complex components.
	BAF	**Melamine:** <1 (Measured) **Cyanuric Acid:** 2.1 (Estimated)	OECD SIDS, 1999a; IUCLID, 2000; EPI	These values are for the individual components.
	Metabolism in Fish	**Melamine:** Uptake, bioaccumulation and elimination study with ^{14}C-melamine in fathead minnow (BCF = 0.48 and 0.26) and rainbow trout (BCF = 0.11, 0.05, 0.03) (Measured)	ECHA, 2011a	Non-guideline studies that support the low bioaccumulation concern for this substance.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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Melamine Polyphosphate

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame-retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with a substance, including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

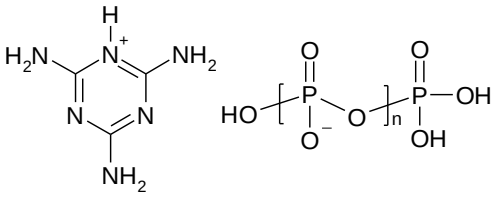
VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from estimation software and professional judgment.

§ Based on analogy to experimental data for a structurally similar compound.

		Human Health Effects											Aquatic Toxicity		Environmental Fate	
Chemical	**CASRN**	**Acute Toxicity**	**Carcinogenicity**	**Genotoxicity**	**Reproductive**	**Developmental**	**Neurological**	**Repeated Dose**	**Skin Sensitization**	**Respiratory Sensitization**	**Eye Irritation**	**Dermal Irritation**	**Acute**	**Chronic**	**Persistence**	**Bioaccumulation**
Melamine Polyphosphate[1]	15541-60-3	L	***M***	***M***	***L*** §	***L***	***L*** §	***M***	L		L	VL	L	L	***H***	***L***

[1] Hazard designations are based upon the component of the salt with the highest hazard designation, including the corresponding free acid or base.

Melamine Polyphosphate



	CAS No. 15541-60-3
	MW: >1,000
	MF: $C_3H_6N_6 \cdot (H_3PO_4)_n$
	Physical Forms: **Neat:** Solid
	Use: Flame retardant

SMILES: n(c(nc(n1)N)N)c1N(H)(H)OP(=O)(O)OP(=O)(O)O (n =1)

Synonyms: Diphosphoric acid, compound with 1,3,5-triazine-2,4,6-triamine; Polyphosphoric acids, compounds with melamine. The CASRN for the compound melamine pyrophosphate is on the TSCA inventory, 15541-60-3. The CASRN 218768-84-4 is associated with the product Melapur 200, not the chemical melamine polyphosphate

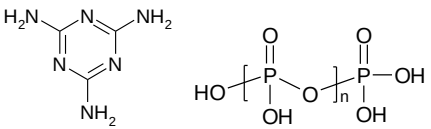
Chemical Considerations: This alternative contains a polymeric moiety. Although the chain length of the polyphosphoric acid is not specified, the smaller, water-soluble polyphosphate ions were used in assessment (generally as the diphosphate ion, n=1). Melamine polyphosphate will freely dissociate under environmental conditions. Measured values from studies on the dissociated components were used to supplement data gaps as appropriate and EPI v 4.0 was used to estimate physical/chemical and environmental fate values in the absence of experimental data. Measured values from experimental studies were incorporated into the estimations.

Polymeric: Yes
Oligomers: Melamine polyphosphate is a complex mixture consisting of melamine and polyphosphate chains of varying length.

Metabolites, Degradates and Transformation Products: Melamine

Analogs: Confidential structurally similar polymers; Polyphosphoric acid (8017-16-1) and melamine (108-78-1) are the dissociated components of this salt
Endpoint(s) using analog values: Reproductive Effects, Neurotoxicity, immunotoxicity

Analog Structure:



Structural Alerts: Aromatic amine, genetic toxicity (U.S. EPA, 2011)
Risk Phrases: Not classified by Annex I Directive 67/548/EEC & IUCLID (Pakalin et al., 2007).
Hazard and Risk Assessments: Australian Safety and Compensation Council National Industrial Chemicals Notification and Assessment Scheme (NICNAS), October 30, 2006 (Australia, 2006); U.S. EPA DfE Alternatives Assessment for Flame Retardants in Printed Circuit Boards, Review Draft, November 8, 2008.
U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.

Melamine Polyphosphate CASRN 15541-60-3			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	> 400 (Measured, Confidential)	Submitted confidential study	Adequate; value for the melamine polyphosphate salt.
	> 400 (Measured)	Australia, 2006	Adequate; value for the melamine polyphosphate salt.
Boiling Point (°C)	>300 (Estimated)	EPI; Professional judgment	As an organic salt, it is expected to decompose before boiling.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	EPI; EPA, 2011	Cutoff value for non volatile compounds according to SF assessment guidance.
Water Solubility (mg/L)	20,000 (Measured, Confidential)	Submitted confidential study	Adequate; value for the melamine polyphosphate salt.
	20,000 (Measured)	Australia, 2006	Adequate.
Log K_{ow}	< -2 (Estimated)	EPI	Cutoff value for highly water soluble substances.
Flammability (Flash Point)	Not highly flammable (Measured, Confidential)	Submitted confidential study	Adequate.
Explosivity	Not a potential explosive (Measured, Confidential)	Submitted confidential study	Adequate.
	Not a potential explosive (Measured)	Australia, 2006	Adequate.
Pyrolysis			No data located.
pH			No data located.
pK_a			No data located.
HUMAN HEALTH EFFECTS			
Toxicokinetics	**No toxicokinetic data located for melamine polyphosphate or polyphosphoric acid; limited data for melamine indicate an elimination phase half-life of 2.7 hours from plasma and 3.0 hours for urine.**		
Dermal Absorption *in vitro*			No data located.
Absorption, Distribution, **Oral, Dermal or Inhaled**	**Melamine polyphosphate:** Low for all routes (Estimated)	Professional judgment	Estimates based on physical/chemical properties.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Metabolism & Excretion		**Melamine:** The elimination phase half-life calculated from plasma data was 2.7 hours, and the urinary half-life was 3.0 hours. The renal clearance was determined to be 2.5 mL/minute (Measured)	Mast et al., 1983	For melamine; adequate, non-guideline study.
		Melamine: Distributed to stomach, small intestine, cecum, and large intestine, and found in blood, and urine of rats	ECHA, 2011b	Study details reported in a secondary source.
Acute Mammalian Toxicity		**LOW: Melamine polyphosphate is expected to be of low hazard for acute toxicity based on experimental evidence for melamine polyphosphate, phosphoric acids and melamine. The weight of evidence indicates that when administered orally and dermally to rats, mice and rabbits, melamine polyphosphate, polyphosphoric acid, and melamine do not produce substantial mortality at levels up to 1,000 mg/kg.**		
Acute Lethality	**Oral**	**Melamine polyphosphate:** Rat (Gavage) LD_{50} >2,000 mg/kg	Ciba, 2005	Sufficient study details reported.
		Melamine polyphosphate: Rat LD_{50} >2,000 mg/kg b.w.	NOTOX B.V., 1998	Limited study details reported.
		Melamine polyphosphate: Rat (Gavage) LD_{50} >2,000 mg/kg (Confidential)	Submitted confidential study	Study details reported in a confidential study.
		Melamine polyphosphate: Rat LD_{50} >2000 mg/kg. (Confidential)	Submitted confidential study	Limited study details reported in a confidential study.
		Polyphosphoric acid: LD_{50} = 4,000 mg/kg (species unknown)	ARZNAD, 1957	Limited study details reported. The test substance was identified as polyphosphates, and was described as containing 1/3 Kurrol's potassium salt and 2/3 pyrophosphate.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Rat LD_{50} = 3,161 mg/kg (male), 3,828 mg/kg (females)	NTP, 1983; Melnick et al., 1984	Sufficient study details reported.
		Melamine: Mouse LD_{50} = 3,296 mg/kg (male), 7,014 mg/kg (female)	NTP, 1983; Melnick et al., 1984	Sufficient study details reported.
		Melamine: Mouse LD_{50} = 4,550 mg/kg	Trochimowicz et al., 2001; American Cyanamid Company, 1955; May, 1979	Limited study details reported.
		Melamine: Rat LD_{50} = 3,160 mg/kg (male) and 3,850 mg/kg (female)	Trochimowicz et al., 2001	Limited study details reported.
		Melamine: Rat LD_{50} >6,400 mg/kg	BASF, 1969	Limited study details reported.
		Melamine: $LD_{50} \approx$ 4,800 mg/kg	Hoechst AG, 1963	Limited study details reported.
	Dermal	**Melamine:** Rabbit LD_{50} > 1,000 mg/L	Unknown, 1990	Limited study details reported.
	Inhalation	**Melamine:** Rat LC_{50} = 3.248 mg/L	Ubaidullajev, 1993	Limited study details reported.
Carcinogenicity		**MODERATE: Estimated based on the dissolution product melamine. There is experimental evidence that oral melamine exposure causes carcinogenicity in animals; however, no data were located to support its carcinogenicity in humans. Tumor formation in animals appeared to happen in a mechanical nature under conditions in which it produced bladder calculi. No carcinogenicity data for melamine polyphosphate were located. IARC classifies melamine as Group 3: *not classifiable as to its carcinogenicity to humans.***		
	OncoLogic Results	**Melamine:** Marginal (Estimated)	OncoLogic, 2005	
	Carcinogenicity (Rat and Mouse)	**Melamine:** Group 3: melamine is not classifiable as to its carcinogenicity to humans; there is inadequate evidence in humans for the carcinogenicity of melamine, and there is sufficient evidence in experimental animals for the carcinogenicity of melamine under conditions in which it produces bladder calculi.	IARC, 1999	IARC classification statement.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Significant formation of transitional cell carcinomas in the urinary bladder of male rats and significant chronic inflammation in the kidney of dosed female rats were observed. Carcinoma formation was significantly correlated with the incidence of bladder stones. A transitional-cell papilloma was observed in the urinary bladder of a single high dose male rat, and compound related lesions were observed in the urinary tract of dosed animals. Based on the mechanical nature of the tumor formation, FDA and EPA considered melamine noncarcinogenic.	NTP, 1983; Huff, 1984; Melnick et al., 1984	Sufficient study details reported.
		Melamine: Increased incidence of acute and chronic inflammation and epithelial hyperplasia of the urinary bladder was observed in male mice. Bladder stones and compound-related lesions were observed in the urinary tract of test animals. Melamine was not considered carcinogenic.	NTP, 1983; Huff, 1984; Melnick et al., 1984	Sufficient study details reported.
		Melamine: Melamine-induced proliferative lesions of the rat urinary tract were directly due to the irritant stimulation of calculi, and not to molecular interactions between melamine or its metabolites with the bladder epithelium.	Okumura et al., 1992	Sufficient study details reported.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Water intake, used as an index of urinary output, was increased by NaCl treatment. Calculus formation resulting from melamine administration was suppressed dose-dependently by the simultaneous NaCl treatment. The main constituents of calculi were melamine and uric acid (total contents 61.1–81.2%). The results indicate that melamine-induced proliferative lesions of the urinary tract of rats were directly due to the irritation stimulation of calculi, and not molecular interactions between melamine itself or its metabolites with the bladder epithelium.	Ogasawara et al., 1995	Sufficient study details reported.
		Melamine: As an initiator, melamine caused no significant increase in papillomas per mouse when compared to controls.	Perrella and Boutwell, 1983	Non-guideline study.
		Melamine: Diffuse papillary hyperplasia of the bladder epithelium and bladder calculi were observed in all melamine treated rats. Elevated spermidine/spermine N1-acetyltransferase activity following melamine treatment was considered to be an indicator of cell proliferation.	Matsui-Yuasa et al., 1992	Non-guideline study.
		Melamine: Decreased antitumor activity was correlated with increasing demethylation; melamine was considered inactive as an antitumor drug.	Rutty and Connors, 1977	Limited study details reported.
		Melamine: In an *in vitro* cytotoxicity study in cultured ADJ/PC6 plasmacytoma ascites tumor cells, the ID_{50} was 470 µg/mL after 72 hours of treatment.	Rutty and Abel, 1980	Limited study details reported.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Combined Chronic Toxicity/ Carcinogenicity	**Melamine:** No effects were observed in rats fed 1,000 ppm of melamine. 4 of the 10 rats fed 10,000 ppm melamine had bladder stones associated with the development of benign papillomas.	Anonymous, 1958	Limited study details reported.
		Melamine: Increased incidence of urinary bladder stones (6/20 rats) was noted in the 10,000 ppm dose group, and was associated with an increase in benign papillomata. The NOAEL was determined to be 1,000 ppm (67 mg/kg).	American Cyanamid Company, 1955	Limited study details reported.
Genotoxicity		**MODERATE: Melamine polyphosphate is estimated to be a moderate hazard concern for genotoxicity based on the data for melamine. For melamine, positive results were observed for *in vivo* chromosome aberration and sister chromatid exchange assays conducted by NTP in 1988 and 1989. Available *in vitro* genotoxicity testing was conducted with metabolic activation systems from the liver. NTP suggests this may not account for potential activation from bladder epithelial cells, which is the target organ. Proposed genotoxicity testing using a metabolic activation system from bladder epithelial cells (NTP, 1983) was never conducted (Personal Communication, 2007; 2008).**		
	Gene Mutation *in vitro*	**Melamine:** Bacterial forward mutation assay: Negative with and without liver activation	Haworth et al., 1983; NCI/NTP, 2007	Sufficient study details reported.
		Melamine: Bacterial forward mutation assay: Negative	Seiler, 1973	Limited study details reported.
		Melamine: Bacterial reverse mutation assay: Negative with and without liver activation	Lusby et al., 1979	Limited study details reported.
		Melamine: Bacterial reverse mutation assay: Negative with and without unspecified metabolic activation	Mast et al., 1982a	Limited study details reported.
		Melamine: *In vitro* mouse lymphoma test: Negative with and without liver activation	McGregor et al., 1988; NCI/NTP, 2007	Sufficient study details reported.
		Melamine: CHO/HGPRT forward mutation assay: Negative with and without liver activation	Mast et al., 1982a	Limited study details reported.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	**Melamine:** *In vitro* chromosomal aberrations test: Negative in CHO with and without liver activation	Galloway et al., 1987; NCI/NTP, 2007	Sufficient study details reported.
		Melamine: *In vitro* sister chromatid exchange assay: Negative in CHO with and without liver activation	Galloway et al., 1987; NCI/NTP, 2007	Sufficient study details reported.
		Melamine: *In vitro* sister chromatid exchange assay: Negative in CHO with and without liver activation	Mast et al., 1982a	Limited study details reported.
	Chromosomal Aberrations *in vivo*	**Melamine:** *In vivo* mouse micronucleus test: The initial test gave a positive trend (P = 0.003) for chromosomal damage; however, both peripheral blood smears and the repeat bone marrow test were negative. The overall conclusion was that melamine does not induce chromosomal damage.	NTP, 1983; Shelby et al., 1993	Sufficient study details reported.
		Melamine: *In vivo* mouse micronucleus test: Negative without activation (Measured)	Mast et al., 1982b	Limited study details reported.
		Melamine: *In vivo* chromosome aberrations test in mice: Positive	NCI/NTP, 2007	Sufficient study details reported.
		Melamine: *In vivo* sister chromatid exchange assay in mice: Positive	NCI/NTP, 2007	Sufficient study details reported.
	DNA Damage and Repair	**Melamine:** *In vivo* and *in vitro* unscheduled DNA synthesis (UDS) test: None of the tested chemicals, including melamine, were genotoxic hepatocarcinogens in the *in vivo* assay, and melamine was negative for UDS in the *in vitro* assay	Mirsalis et al., 1983	Limited study details reported.
		Melamine: SOS/*umu* test: Negative for its ability to result in DNA damage and induce the expression of the *umu* operon	Reifferscheid and Heil, 1996	Non-guideline study.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: DNA synthesis-inhibition test in Hela S3 cells: Inhibits DNA synthesis by 50% at greater than 300 μM	Heil and Reifferscheid, 1992	Limited study details reported.
	Other	**Melamine:** Sex-linked recessive lethal/reciprocal translocation: Results were considered equivocal based on 0.18% and 0.36% total lethal following oral and injection exposure, respectively, compared to control total lethal of 0.07% for oral and 0.09% for injection	NCI/NTP, 2007	Sufficient study details reported.
		Melamine: *Drosophila* Muller-5 test: Negative for mutagenicity	Rohrborn, 1959	Limited study details reported.
		Melamine: *Drosophila melanogaster* Sex-linked recessive lethal: No mutagenic effects were observed	Luers and Rohrborn, 1963	Limited study details reported.
		Melamine: *In vitro* flow cytometric DNA repair assay: Negative for genotoxic effects	Seldon et al., 1994	Non-guideline study.
		Melamine: Microscreen assay: Positive for genetic toxicity in *E. coli* WP2 cells	Rossman et al., 1991	Non-guideline study.
		Melamine: Growth and genotoxic effects to bacteria (*Salmonella typhimurium*) and yeast (*Saccharomyces cerevisiae*): Non-mutagenic in *S.typhimurium* with or without S-9 mix. The growth of eight out of nine strains tested was delayed by 10 mM melamine during 24 hour cultivation. *S.cerevisiae* strain was tested, and did not recover its growth following 48 hour cultivation	Ishiwata et al., 1991	Limited study details reported.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Reproductive Effects		**LOW: Estimated based on analogy to structurally similar polymers and professional judgment.**		
	Reproduction/ developmental toxicity screen			No data located.
	Combined repeated dose with reproduction/developmental toxicity screen			No data located.
	Reproduction and fertility effects	**Melamine:** Reproductive dysfunction was observed at 0.5 mg/m^3 and included effects on spermatogenesis (genetic material, sperm morphology, motility, and count), effects on the embryo/fetus (fetal death), pre-implantation mortality (reduction in the number of implants per female), and total number of implants per corpora lutea.	Ubaidullajev, 1993	Study details, if present, were not translated into English.
		Melamine: There were no treatment-related macroscopic or microscopic effects on mammary glands, ovaries, prostate, seminal vesicles, testes and uterus in rats and mice in a 13 week study.	OECD, 1999	Study details, including administered dose information, were not provided.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**LOW: Melamine polyphosphate is estimated to be of low hazard concern for developmental effects based on the data for melamine. For melamine, no adverse effects on gestational parameters, no signs of developmental toxicity.**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Prenatal Development	**Melamine:** Signs of maternal toxicity at 136 mg/kg b.w. included decreased body weight and feed consumption, hematuria (23/25 rats), indrawn flanks (7/25 rats), and piloerection (1/25 rats). No adverse effects on gestational parameters and no signs of developmental toxicity were noted. NOAEL ≥1,060 mg/kg-day	Hellwig et al., 1996	Sufficient study details reported.
	Postnatal Development	**Melamine:** Only minor effects on the fetuses or litters, including a non-significant increase in resorptions in the group treated on the 4th and 5th days of gestation, were observed.	Thiersch, 1957	Sufficient study details were not available.
Neurotoxicity		**LOW: Based on professional judgment through analogy to structurally similar polymers.**		
	Neurotoxicity Screening Battery (Adult)	Potential for neurotoxicity is expected to be low. (Estimated)	Professional judgment	Estimated based on analogy and professional judgment.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects		**MODERATE: Melamine polyphosphate is expected to be a moderate hazard for repeated dose effects based on the data for melamine. Stones and diffuse epithelial hyperplasia in the urinary bladders were observed in male rats at doses as low as 700 ppm (72 mg/kg/day).**		
		Polyphosphoric Acid: Rat Repeated-Dose Toxicity Study: An oral repeated-dose toxicity test in rats resulted in a TD_{Lo} of 450 mg/kg. The test substance was identified as polyphosphates, and was described as containing 1/3 Kurrol's potassium salt and 2/3 pyrophosphate. Toxic effects included changes in liver weight, changes in tubules (including acute renal failure, acute tubular necrosis), and weight loss or decreased weight gain.	ARZNAD, 1957	Sufficient study details were not available.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Rat 28-day dietary toxicity study: Clinical signs included a dose-related increase in pilo-erection, lethargy, bloody urine spots in the cage and on the pelage of animals, and chromodacryorrhea. The incidence of urinary bladder calculi and urinary bladder hyperplasia in treated animals was dose dependent, with a significant relationship between the calculi and hyperplasia. Calculi composition indicated the presence of an organic matrix containing melamine, phosphorus, sulfur, potassium, and chloride. Crystals of dimelamine monophosphate were identified in the urine. The NOAEL was estimated to be 2,000 ppm (240 mg/kg/day), excluding the observed increase in water consumption and the incidence of crystalluria. LOAEL was determined to be 4,000 ppm (475 mg/kg/day) based on the formation of calculus.	RTI, 1983	Sufficient study details reported.
		Melamine: Rabbit and dog 28-day dietary toxicity study: No significant rise in the body temperature of rabbits was noted. Gross histological examination of the heart, lung, liver, spleen, thyroid, pancreas, intestines, kidneys and bladder did not show pathological changes. A zone of fat was found in the inner part of the renal cortex in two dogs, but also in the kidneys of 3 control dogs.	Lipschitz and Stokey, 1945	Sufficient study details were not available.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Rat 28-day dietary toxicity study: Incidence and size of bladder stones were directly related to the amount of substance administered. The larger stones were found to be unchanged melamine in a matrix of protein, uric acid and phosphate. Lowest effective dose: 1,500 ppm (~125 mg/kg) in males.	American Cyanamid Company, 1984	Sufficient study details were not available.
	Chronic	**Melamine:** Rat 90-day dietary toxicity study: one male rat receiving 18,000 ppm and two males receiving 6,000 ppm died. Mean body weight gain and feed consumption were reduced. Stones and diffuse epithelial hyperplasia in the urinary bladders were observed in male rats of all treatment groups. Focal epithelial hyperplasia was observed in only 1 male. A second and third 13-week repeated dose toxicity study was conducted in rats at a dose range of 750 to 18,000 ppm; bladder stones were observed at all dose levels. LOAEL = 700 ppm (72 mg/kg/day)	NTP, 1983; Melnick et al., 1984; ECHA 2011b	Sufficient study details reported.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Mouse 90-day Dietary Toxicity Study: A single female mouse died after receiving 9,000 ppm. Mean body weight gain relative to controls was depressed. The incidence of mice with bladder stones was dose-related and was greater in males than in females. Sixty percent of mice having bladder ulcers also had urinary bladder stones. Bladder ulcers were multifocal or associated with inflammation (cystitis). Epithelial hyperplasia and bladder stones were observed together in 2 mice. Also, epithelial cell atypia was seen. NOAEL: 6,000 ppm (600 mg/kg-day). LOAEL: 9,000 ppm (900 mg/kg-day)	NTP, 1983; Melnick et al., 1984	Sufficient study details reported.
		Melamine: Increased incidence of acute and chronic inflammation and epithelial hyperplasia of the urinary bladder was observed in mice following oral (feed) exposure for up to 103 weeks. There was also increased incidence of bladder stones in male mice. LOAEL = 2,250 ppm (lowest dose tested)	NTP, 1983; ECHA, 2011a	Repeated dose effects described in a carcinogenicity bioassay study.
		Melamine: Dog 1-year dietary toxicity study: crystalluria started 60 to 90 days into treatment, and persisted during the study period. No other effects attributable to melamine were observed.	American Cyanamid Company, 1955	Sufficient study details were not available.
		Melamine: Rat 30-month dietary toxicity study: neither accumulation of calculi nor any treatment-related urinary bladder lesions were found.	Mast et al., 1982c	Sufficient study details were not available.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Rat 24 to 30-month dietary toxicity study: a dose related trend for dilated glands in glandular gastric mucosa and inflammation in non glandular gastric mucosa was observed. Urinary bladder calculi formation was not observed.	American Cyanamid Company, 1983	Sufficient study details were not available.
Skin Sensitization		**LOW: Melamine polyphosphate is not expected to be a skin sensitizer based on the data for melamine.**		
	Skin Sensitization	**Melamine:** No evidence of primary dermal irritation or sensitization in a human patch test	American Cyanamid Company, 1955; Trochimowicz et al., 2001	Limited study details reported.
		Melamine: Non-sensitizing to guinea pigs	Fasset and Roudabush, 1963/1981; Trochimowicz et al., 2001	Limited study details reported.
Respiratory Sensitization		**No data located**.		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Melamine polyphosphate is slightly irritating to eyes.**		
	Eye Irritation	**Melamine polyphosphate:** Slightly irritating	NOTOX B.V., 1998	Limited study details reported.
		Melamine polyphosphate: Slightly irritating	Submitted confidential study	Limited study details reported.
		Melamine: Non-irritating to rabbit eyes	BASF, 1969	Limited study details reported.
		Melamine: Non-irritating to rabbit eyes following 0.5 mL of 10% melamine	American Cyanamid Company, 1955; Trochimowicz et al., 2001	Limited study details reported.
		Melamine: Mild irritant to rabbit eyes following exposure to 30 mg of dry powder	American Cyanamid Company, 1955; Trochimowicz et al., 2001	Limited study details reported.
		Melamine: Slightly irritating to rabbit eyes	Marhold, 1972	Limited study details reported.
Dermal Irritation		**VERY LOW: Melamine polyphosphate is not a skin irritant.**		
	Dermal Irritation	**Melamine polyphosphate:** Not irritating	NOTOX B.V., 1998	Limited study details reported.
		Melamine polyphosphate: Not irritating	Submitted confidential study	Limited study details reported.
		Melamine: Not irritating to rabbit skin	Rijcken, 1995	OECD 404 guideline study
		Melamine: Not irritating to rabbit skin	BASF, 1969	Limited study details reported.
		Melamine: Not irritating to rabbit skin	American Cyanamid Company, 1955; Trochimowicz et al., 2001	Limited study details reported.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: Not irritating to rabbit skin	Fasset and Roudabush, 1963/1981; Trochimowicz et al., 2001	Limited study details reported.
Endocrine Activity		**There were insufficient data located to describe the effect of melamine polyphosphate on the endocrine system. In one study, melamine did not exhibit estrogenic activity *in vitro* in a yeast two-hybrid assay.**		
		Melamine: Showed no estrogenic activity (no change in B-galactosidase activity) in an *in vitro* yeast two-hybrid assay in *Saccharomyces cerevisia* Y 190	ECHA, 2011	No guideline followed.
Immunotoxicity		**Potential for immunotoxic effects based on analogy to structurally similar polymers.**		
	Immune System Effects	**Melamine:** Did not inhibit the mitogenesis of B- and T- lymphocytes in an *in vitro* mouse lymphocyte mitogenesis test.	ECHA, 2011b	Unclear how well mitogenesis test assesses immunotoxicity of chemicals.
ECOTOXICITY				
ECOSAR Class		Anilines (amino-meta), Triazines		
Acute Toxicity		**LOW: Melamine polyphosphate is expected to be of low hazard for acute toxicity to aquatic organisms based on experimental data for melamine polyphosphate and experimental data for melamine. For melamine, the weight of evidence suggests that the acute values are >100 mg/L. For melamine polyphosphate, no effects were observed at the highest concentration tested (3.0 mg/L). Melamine polyphosphate does not cause eutrophication.**		
Fish LC_{50}		**Melamine polyphosphate:** Freshwater fish 96-hour LC_{50} = 100 mg/L (Experimental)	Ciba, 2005	Reported in a secondary source, study details and test conditions were not reported.
		Melamine: *Leuciscus idus melanotus* 48-hour LC_{50} >500 mg/L (Experimental)	SIDS, 1999	Study details reported in secondary source.
		Melamine: *Oryzias latipes* 48-hour LC_{50} = 1000 mg/L (Experimental)	SIDS, 1999	Study details reported in secondary source.
		Melamine: *Poecilia reticulata* 96-hour LC_{50} >3,000 mg/L (Experimental)	SIDS, 1999	Study details reported in secondary source.
		Melamine: *Poecilia reticulata* 4,400 mg/L dose lethal to <10% (Experimental)	SIDS, 1999	Study details reported in secondary source.

Melamine Polyphosphate CASRN 15541-60-3			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine: Fish 96-hour LC_{50} = 2,680 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	EPI	
	Melamine: Fish 96-hour LC_{50} = 391 mg/L (Estimated) ECOSAR: Melamines	EPI	
	Melamine: Fish 96-hour LC_{50} = 14,272 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
Daphnid LC_{50}	**Melamine polyphosphate:** Daphnia magna 48-hour EC_{50} >100 mg/L	Ciba, 2005	Reported in a secondary source, study details and test conditions were not reported.
	Melamine: *Daphnia magna* 48-hour LC_{50} > 2000 mg/L (Experimental)	SIDS, 1999	Study details reported in secondary source.
	Melamine: Daphnid 48-hour LC_{50} = 6.23 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	EPI	
	Melamine: Daphnid 48-hour LC_{50} = 144.34 mg/L (Estimated) ECOSAR: Melamines	EPI	
	Melamine: Daphnid 48-hour LC_{50} = 4,805 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
Green Algae EC_{50}	**Melamine polyphosphate:** *Selenastrum capricornutum* 96-hour EC_{50} >3.0 mg/L (Experimental, Confidential); 96-hour NOEC = 3.0 mg/L (Experimental, Confidential)	Submitted confidential study	No effects observed at highest concentration tested.
	Melamine polyphosphate: *Selenastrum capricornutum* 96-hour EC_{50} >3.0 mg/L (Experimental); 96-hour NOEC = 3.0 mg/L (Experimental)	Australia, 2006	Reported in a secondary source, study details and test conditions were not provided; no effects observed at highest concentration tested.

Melamine Polyphosphate CASRN 15541-60-3			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine polyphosphate: In a 96-hour control growth test (*Selenastrum capricornutum*), melamine polyphosphate causes increased algal growth, but growth is 95% less than growth in standard medium with adequate phosphorous. This indicates that melamine polyphosphate is not a good source of phosphorous for algal growth and does not cause eutrophication. (Experimental, Confidential)	Submitted confidential study	Sufficient study details reported in a confidential study.
	Melamine: Green algae 96-hour EC_{50} = 2.79 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	EPI	
	Melamine: Green algae 96-hour EC_{50} = 325 mg/L (Estimated) ECOSAR: Melamines	EPI	
	Melamine: Green algae 96-hour EC_{50} = 4,396 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Melamine: *Scenedesmus pannonicus* 4-day EC_{50} = 940 mg/L (Experimental); 4-day NOEC = 320 mg/L (Experimental)	SIDS, 1999	Reported in a secondary source, study details and test conditions were not provided.
Chronic Aquatic Toxicity	**LOW: Melamine polyphosphate is expected to be of low hazard for chronic toxicity to aquatic organisms based on experimental data for melamine. For melamine, the weight of evidence suggests that the chronic values are >10 mg/L.**		
Fish Chronic Value (ChV)	**Melamine:** *Jordanella floridae* 35-day NOEC ≥1,000 mg/L (Experimental)	SIDS, 1999	Reported in a secondary source, study details and test conditions were not provided.
	Melamine: *Salmo gairdneri* NOEC (macroscopic) = 500 mg/L (Experimental); NOEC (microscopic) <125 mg/L (Experimental)	SIDS, 1999	Reported in a secondary source, study details and test conditions were not provided.

Melamine Polyphosphate CASRN 15541-60-3			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Melamine: Fish ChV = 263 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	EPI	The toxicity value was estimated through application of acute-to-chronic ratios.
	Melamine: Fish ChV = 1,102 mg/L (Estimated) ECOSAR: Melamines	EPI	
	Melamine: Fish ChV = 1,076 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
Daphnid ChV	**Melamine:** *Daphnia magna* 21-day LC_{50} = 32-56 mg/L, 21-day LC_{100} = 56 mg/L, 21day NOEC = 18 mg/L (Experimental)	SIDS, 1999	Reported in a secondary source, study details and test conditions were not provided.
	Melamine: Daphnid ChV = 0.078 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	EPI	
	Melamine: Daphnid ChV = 14.85 mg/L (Estimated) ECOSAR: Melamines	EPI	The toxicity value was estimated through application of acute-to-chronic ratios.
	Melamine: Daphnid ChV = 343.93 mg/L (Estimated) ECOSAR class: Neutral organics	EPI	
Green Algae ChV	**Melamine**: Green algae ChV = 0.70 mg/L (Estimated) ECOSAR: Anilines (amino-meta)	EPI	The toxicity value was estimated through application of acute-to-chronic ratios.
	Melamine: Green algae ChV = 81.26 mg/L (Estimated) ECOSAR: Melamines	EPI	
	Melamine: Green algae ChV = 313.17 mg/L (Estimated) ECOSAR: Neutral organics	EPI	

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**Melamine polyphosphate has a high measured water solubility of 20 g/L and its Henry's Law Constant and vapor pressure are below cutoff values. It is expected to partition predominately to water and soil. It may migrate from soil into groundwater. As a salt, volatilization from either wet or dry surfaces is not expected to be an important fate process.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	EPI; Professional judgment	Cutoff value for nonvolatile compounds.
	Sediment/Soil Adsorption/ Desorption Coefficient – K_{oc}	**Melamine polyphosphate:** 13 (Estimated)	EPI	
	Level III Fugacity Model	**Melamine polyphosphate:** Air = 0% Water = 37% Soil = 63% Sediment = 0% (Estimated)	EPI	
Persistence		**HIGH: Melamine polyphosphate is expected to show high persistence in the environment based on the data for melamine, which is expected to be fully dissociated under environmental conditions. The weight of evidence suggests that melamine will biodegrade, but not rapidly. Degradation of melamine or its cation by hydrolysis or direct photolysis is not expected to be significant as the functional groups present on this molecule do not tend to undergo these reactions under environmental conditions. Polyphosphoric acid is expected to have low persistence in the environment. The weight of evidence suggests that polyphosphoric acid will hydrolyze under environmental conditions. The phosphates formed are expected to participate in natural cycles and be readily assimilated.**		
Water	**Aerobic Biodegradation**	**Melamine polyphosphate:** Weeks (Primary survey model) Months (Ultimate survey model)	EPI	

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Melamine: 16% removal after 20 days with activated sludge, 14% removal after 10 days with adapted sludge (Measured)	SIDS, 1999	These values are for the dissociated component, melamine. Reported in a secondary source, study details and test conditions were not provided.
		Melamine: 0% removal after 28 days with activated sludge (Measured)	SIDS, 1999	
		Melamine: 0% removal after 14 days with activated sludge (Measured)	SIDS, 1999	
		Melamine: <30% removal after 14 days with activated sludge (Measured)	SIDS, 1999	
		Melamine: <1% removal after 5 days with an adapted inoculum (Measured)	IUCLID, 2000a	
		Melamine: 0% removal after 14 days with activated sludge (Measured)	IUCLID, 2000a	
		Melamine: <30% removal after 14 days with activated sludge (Measured)	IUCLID, 2000a	
		Melamine: <20% removal after 20 days, 14% removal after 10 days with adapted inoculum (Measured)	IUCLID, 2000a	
	Volatilization Half-life for Model River	**Melamine polyphosphate:** >1 year (Estimated)	EPI	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	**Melamine polyphosphate:** >1 year (Estimated)	EPI	Based on the magnitude of the estimated Henry's Law Constant.
Soil	**Aerobic Biodegradation**	**Melamine:** Not readily biodegradable: 0% biodegradation detected after 2 weeks with 100 ppm in 30 ppm activated sludge (OECD TG 301C) (Measured); 0% degradation after 28 days with 100 mg DOC/L in activated sludge (Zahn-Wellens test, OECD 302B) (Measured)	MITI, 1998; OECD SIDS, 1999	Adequate values from guideline studies for the dissociated component, melamine.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Anaerobic Biodegradation	**Melamine:** 0-8.9% nitrification was observed after 28 days incubation with bacteria in Webster silty clay loam under anaerobic conditions (Measured)	IUCLID, 2000a	This value is for the dissociated component, melamine. Reported in a secondary source, study details and test conditions were not provided.
	Soil Biodegradation w/ Product Identification	**Melamine:** Nitrification of melamine occurs in soil at a low rate (0.7% organic N found as NO_3-N in week 10, and 0 % in week 28). (Measured)	ECHA, 2011a, 2011b	Non guideline studies for the dissociated component, melamine.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	**Melamine polyphosphate:** 21 days (Estimated)	EPI	
Reactivity	**Photolysis**	**Melamine polyphosphate:** Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
	Hydrolysis	**Polyphosphoric acid:** The half-life for the hydrolysis to phosphoric acid is several days at 25°C (Measured)	Kirk-Othmer, 2005	This value is for the dissociated component, polyphosphoric acid. These studies indicate polyphosphoric acid would undergo hydrolysis under environmental conditions to phosphate ions. Reported in a secondary source, study details and test conditions were not provided.
		Polyphosphoric acid: Hydrolysis occurs in 2 months at 20°C (Measured)	IUCLID, 2000b	This value is for the dissociated component, polyphosphoric acid. Reported in a secondary source, study details and test conditions were not provided available.

Melamine Polyphosphate CASRN 15541-60-3				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Environmental Half-life		**Melamine polyphosphate:** 120 days (Estimated)	EPI; PBT Profiler	Half-life estimated for the predominant compartment, as determined by EPI and the PBT Profiler methodology.
Bioaccumulation		**LOW: Based on the relatively high water solubility of melamine polyphosphate (20 g/L) and an estimated BCF of 3.2. In addition, the experimental bioconcentration values for the melamine component are low, BCF <3.8, and estimated BAF <1.**		
	Fish BCF	**Melamine polyphosphate:** 3.2 (Estimated)	EPI	
		Melamine: <0.38 in carp (*Cyprinus carpio*) after 6 weeks at 2.0 ppm concentration; <3.8 in carp (*Cyprinus carpio*) after 6 weeks at 0.2 ppm concentration (OECD 302B) (Measured)	MITI, 1998	Adequate values from guideline studies for the dissociated component, melamine.
	BAF	**Melamine polyphosphate:** 0.9 (Estimated)	EPI	
		Melamine: <1 (Measured)	SIDS, 1999; IUCLID, 2000a	This value is for the dissociated component, melamine.
	Metabolism in Fish	**Melamine:** Uptake, bioaccumulation and elimination study with ^{14}C-melamine in fathead minnow and rainbow trout: BCFs <1 (Measured)	ECHA, 2011a, 2011b	Non guideline studies that support the low potential for bioaccumulation of this substance.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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N-alkoxy Hindered Amine Reaction Products

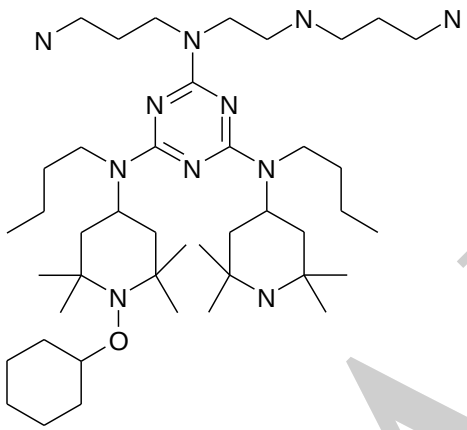
Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from estimation software and professional judgment.
‡ The highest hazard designation of any of the oligomers with MW <1,000

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
N-alkoxy Hindered Amine Reaction Products	191680-81-6	L	*M*	L	*H*	*H*	*L*	*H*	L		L	VL	*H*	*H*	H	*H*‡

N-alkoxy Hindered Amine Reaction Products



Representative Structure

CASRN: 191680-81-6

MW: >1,300 (92%);
670-1,300 (3%);
<670 (5%)

MF:

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: N4C(N(CCNCCCN)CCCN)=NC(N(C2CC(C)(C)N(OC3CCCCC3)C(C)(C)C2)CCCC)=NC=4N(C1CC(C)(C)NC(C)(C)C1)CCCC (Representative Structure)

Synonyms: 1,3-Propanediamine, N1,N1'-1,2-ethanediylbis-, reaction products with cyclohexane and peroxidized N-butyl-2,2,6,6-tetramethyl-4-piperidinamine-2,4,6-trichloro-1,3,5-triazine reaction products (TSCA Inventory); Flamestab Nor 116

Chemical Considerations: This alternative is a polymer. The structure shown is the simplest depiction of an oligomer with a MW <1,000 (approximately 770) that includes all combinations of monomers. This review assesses oligomers with a MW <1,000 using a representative structure. The representative structure lies within the domain of the available estimation methods. EPI v4.0 estimation methods were used for physical/chemical and environmental fate values in the absence of experimental data. The higher MW oligomers with a MW >1,000 are assessed together using the SF polymer assessment criteria (U.S. EPA, 2010a).

Polymeric: Yes **Oligomers:** The MF and MW of this polymer are variable; approximately 90% of the oligomers in this polymer have a MW >1,300 (NICNAS, 2001). The mixture is based on a substituted aliphatic tetra amine, where the substituents on the amine groups are variable. The presence of material in the commercial product with a MW <670 is likely the result of unchanged starting materials.	
Metabolites, Degradates and Transformation Products: None	
Analog: No analog **Endpoint(s) using analog values:** Not applicable	**Analog Structure:** Not applicable
Structural Alerts: Hindered amines (U.S. EPA, 2010b)	
Risk Phrases: Not classified by Annex VI Regulation (European Commission) No 1272/2008 (ESIS, 2011).	
Hazard and Risk Assessments: This polymer has been assessed by NICNAS (NICNAS, 2001).	
U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory and is a commenced Premanufacture Notice substance.	

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	113–121 softening point (Measured)	Ciba Additives, 1997b	Value is a result from DSC analysis on the commercial product, with a reported endotherm trough at 120.43°C. The value of 113°C likely corresponds to a softening point for the polymer.
Boiling Point (°C)	Decomposes (Measured)	Ciba Additives, 1997a	The commercial product was found to decompose without boiling at 260°C at a reduced pressure of 6 kPa.
	>300 (Estimated)	EPI; EPA, 1999	Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. Cutoff value according to HPV assessment guidance.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	EPI; EPA, 2010a	Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. Cutoff value according to SF polymer assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	EPI; EPA, 1999	Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. Cutoff value according to HPV assessment guidance.

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Log K_{ow}		>10 (Estimated)	EPI; EPA, 2011	Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. Cutoff value according to SF assessment guidance.
Flammability (Flash Point)		>110°C (Measured)	NICNAS, 2001	Sufficient details were not available to assess the quality of this study.
Explosivity		Not explosive EEC method A.14 (Measured)	NICNAS, 2001	Adequate; guideline study.
Pyrolysis				No data located.
pH				No data located.
pK_a		2.4 to 10.2 (Estimated)	NICNAS, 2001	Inadequate. Compound only contains basic functional groups.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**As a neat material, N-alkoxy hindered amine reaction products is estimated to not be absorbed by any route of exposure. This compound is expected to have poor absorption through all routes when in solution. This material is predominately a polymer with a MW >1,000 however at present there is no MW cutoff for the hindered amine category of new chemicals.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	Not absorbed by any route as a neat material; poor absorption for all routes when in solution	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/chemical properties.
Acute Mammalian Toxicity		**LOW: Based on an acute oral LD_{50} >5,000 mg/kg and an acute dermal LD_{50} >2,000 mg/kg for rats.**		
Acute Lethality	**Oral**	Rat Oral LD_{50} >5,000 mg/kg bw	NICNAS, 2001	Reported in a secondary source. Guideline study (OECD 401, limit test).
	Dermal	Rat Dermal LD_{50} >2,000 mg/kg bw	NICNAS, 2001	Reported in a secondary source. Guideline study (OECD 402, limit test).
	Inhalation			No data located.

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Carcinogenicity		**MODERATE: There is uncertainty due to lack of data for this substance. EPA does not expect this substance to be carcinogenic however such effects cannot be ruled out.**		
	OncoLogic Results			This polymer is not amenable to available estimation methods.
	Carcinogenicity (Rat and Mouse)			No data located.
	Combined Chronic Toxicity/ Carcinogenicity			No data located.
Genotoxicity		**LOW: N-alkoxy hindered amine reaction products did not induce gene mutations in *Salmonella typhimurium* or *Escherichia coli* and did not induce chromosomal aberrations in Chinese hamster ovary (CHO) cells in the presence and absence of metabolic activation.**		
	Gene Mutation *in vitro*	Negative for gene mutations in *Salmonella typhimurium* strains TA1535, TA1537, TA98, TA100 and *E. coli* strain WP2uvrA with and without metabolic activation.	NICNAS, 2001	Reported in a secondary source. Guideline study (OECD 471, bacterial reverse mutation test).
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	Negative for chromosomal aberrations in CHO cells with and without metabolic activation. No evidence of clastogenicity.	NICNAS, 2001	Reported in a secondary source. Guideline study (OECD 473, *in vitro* mammalian chromosomal aberration test).
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Reproductive Effects		**HIGH: Estimated potential for reproductive effects based on analogy to other hindered amines similar in structure.**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Reproduction and Fertility Effects	Toxicity to male reproductive system (Estimated by analogy)	Professional judgment, TSCA New Chemicals Program – Chemical Categories for hindered amines	Estimated based on analogy to hindered amines similar in structure.
Developmental Effects		**HIGH: Estimated potential for developmental effects based on analogy to other hindered amines similar in structure.**		
	Reproduction/ Developmental Toxicity Screen	Delayed skeletal maturation LOAEL = 1,200 mg/kg/day (Estimated by analogy)	Professional judgment	Estimated based on analogy to hindered amines similar in structure.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Prenatal Development			No data located.
	Postnatal Development			No data located.
Neurotoxicity		**LOW: Estimated not to have potential for neurotoxicity based on expert judgment. No data located.**		
	Neurotoxicity Screening Battery (Adult)	No potential for neurotoxicity (Estimated)	Expert judgment	Estimated based on expert judgment.

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects		**HIGH: Estimated potential for repeated dose effects based on analogy to other hindered amines similar in structure. Experimental data reported that N-alkoxy hindered amine reaction products did not produce adverse effects in a 28-day oral gavage study in rats at oral doses up to 1,000 mg/kg/day; however uncertainty remains for exposure of longer duration.**		
		Toxicity to liver, blood, and gastrointestinal tract (Estimated by analogy)	Professional judgment, TSCA New Chemicals Program – Chemical Categories for hindered amines	Estimated based on analogy hindered amines similar in structure.
		28-day oral gavage study in Sprague-Dawley rats. No treatment-related clinical effects or changes in clinical chemistry, hematology, urinalysis or organ weight. NOAEL = 1,000 mg/kg/day LOAEL = not established as highest dose tested did not produce adverse effects	NICNAS, 2001	Reported in a secondary source. Guideline study (OECD 407). The hindered amines category suggests need for a 90-day oral test.
Skin Sensitization		**LOW: N-alkoxy hindered amine reaction products did not produce skin sensitization in an experimental study in guinea pigs.**		
	Skin Sensitization	No evidence of sensitization, guinea pig	NICNAS, 2001	Reported in a secondary source. Guideline study (OECD 406).
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: N-alkoxy hindered amine reaction products, was slightly irritating to rabbit eyes with clearing within 24 hours.**		
	Eye Irritation	Slightly irritating, rabbit. Most symptoms cleared in 24 hours or less. Redness persisted for 48 hours.	NICNAS, 2001	Reported in a secondary source. Guideline study (OECD 405, acute eye irritation/corrosion).
Dermal Irritation		**VERY LOW: N-alkoxy hindered amine reaction products, is not irritating to rabbit skin.**		
	Dermal Irritation	Non-irritating, rabbit	NICNAS, 2001	Reported in a secondary source. Guideline study (OECD 4014, acute dermal irritation/corrosion).

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Endocrine Activity		**No data located.**		
				No data located.
Immunotoxicity		**Estimated potential for immunotoxic effects based on analogy to other hindered amines similar in structure.**		
	Immune System Effects	Effects on thymus, spleen, lymph and nodes (Estimated by analogy)	Professional judgment, TSCA New Chemicals Program – Chemical Categories	Estimated based on analogy hindered amines similar in structure.
ECOTOXICITY				
ECOSAR Class		Polycationic Polymers; Aliphatic Amines; Triazines		
Acute Toxicity		**HIGH: Based on estimated acute aquatic toxicity values for fish, daphnid, and green algae using polycationic polymer SAR.**		
Fish LC_{50}		*Pimephales promelas* 96-hour LC_{50} >0.268 mg/L, NOEC = 0.268 mg/L (48-hour static-renewal, mean measured)	NICNAS, 2001	Reported in a secondary source. Guideline study (OECD TG 203); reported values are greater than the water solubility; no effects at saturation (NES) were observed for this endpoint.
		Fish 96-hour LC_{50} = 0.28 mg/L (Estimated)	EPI	Predictions based on SARs for polycationic polymers with >3.5% amine-N.
Daphnid LC_{50}		Daphnia 48-hour EC_{50} >0.312 mg/L, NOEC = 0.312 mg/L (24- hour static-renewal, mean measured)	NICNAS, 2001	Reported in a secondary source. Guideline study (OECD TG 202); reported values are greater than the water solubility; NES were observed for this endpoint.
		Daphnid 48-hour LC_{50} = 0.1 mg/L (Estimated)	Professional judgment	Predictions based on SARs for polycationic polymers with >3.5% amine-N.
Green Algae EC_{50}		Green Algae (*Pseudokirchneriella subcapitata)* 72-hour EbC_{50} >0.083 mg/L, NOEC = 0.083 mg/L(static, measured at study termination)	NICNAS, 2001	Reported in a secondary source. Guideline study (OECD TG 201); reported values are greater than the water solubility; NES were observed for this endpoint.

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Green algae 96-hour EC_{50} = 0.04 mg/L (Estimated)	Professional judgment	Predictions based on SARs for polycationic polymers with >3.5% amine-N.
Chronic Aquatic Toxicity	**HIGH: Based on estimated chronic aquatic toxicity values for fish, daphnid, and green algae using polycationic polymer SARs.**		
Fish ChV	Fish ChV = 0.016 mg/L (Estimated)	Professional judgment	Predictions based on SARs for polycationic polymers with >3.5% amine-N.
	ChV = 5.31×10^{-5} mg/L (ECOSAR Estimation, Class: Aliphatic amines)	EPI	NES: Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. The log K_{ow} of 10.22 for this chemical exceeds the SAR limitation of 8.0; NES are predicted for these endpoints. The higher oligomers outside the domain of the estimation method are anticipated to display NES.
	Fish ChV = 5.19×10^{-6} mg/L (ECOSAR Estimation, Class: Triazines)	EPI	NES: Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. The log K_{ow} of 10.22 for this chemical exceeds the SAR limitation of 8.0; NES are predicted for these endpoints The higher oligomers outside the domain of the estimation method are anticipated to display NES.

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Fish ChV = $5.19x10^{-6}$ mg/L (ECOSAR Estimation, Class: Neutral organics)	EPI	NES: Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. The log K_{ow} of 10.22 for this chemical exceeds the SAR limitation of 8.0; NES are predicted for these endpoints The higher oligomers outside the domain of the estimation method are anticipated to display NES.
Daphnid ChV	ChV = 0.014 mg/L (ECOSAR Estimation, Class: Aliphatic amines)	EPI	NES: Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. The log K_{ow} of 10.22 for this chemical exceeds the SAR limitation of 8.0; NES are predicted for these endpoints The higher oligomers outside the domain of the estimation method are anticipated to display NES.
	ChV = $4.67x10^{-5}$ mg/L (ECOSAR Estimation, Class: Triazines)	EPI	NES: Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. The log K_{ow} of 10.22 for this chemical exceeds the SAR limitation of 8.0; NES are predicted for these endpoints The higher oligomers outside the domain of the estimation method are anticipated to display NES.
	ChV = 0.007 mg/L (Estimated)	Professional judgment	Predictions based on SARs for polycationic polymers with >3.5% amine-N.

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Saltwater Invertebrate ChV	ChV = 0.014 mg/L (ECOSAR Estimation, Class: Aliphatic amines)	EPI	NES: Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. The log K_{ow} of 10.22 for this chemical exceeds the SAR limitation of 8.0; NES are predicted for these endpoints The higher oligomers outside the domain of the estimation method are anticipated to display NES.
Green Algae ChV	ChV = 0.000234 mg/L (ECOSAR Estimation, Class: Aliphatic amines)	EPI	NES: Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. The log K_{ow} of 10.22 for this chemical exceeds the SAR limitation of 7.0; NES are predicted for these endpoints The higher oligomers outside the domain of the estimation method are anticipated to display NES.
	ChV = 0.002 mg/L (ECOSAR Estimation, Class: Triazines)	EPI	NES: Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. The log K_{ow} of 10.22 for this chemical exceeds the SAR limitation of 7.0; NES are predicted for these endpoints. The higher oligomers outside the domain of the estimation method are anticipated to display NES.
	ChV = 0.02 mg/L (Estimated)	Professional judgment	Predictions based on SARs for polycationic polymers with >3.5% amine-N.

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**Based on the Level III fugacity models incorporating the available property data, N-alkoxy hindered amine reaction products is expected to partition primarily to soil and sediment. This compound is expected to be immobile in soil based on its estimated K_{oc}. Leaching of N-alkoxy hindered amine reaction products through soil to groundwater is not expected to be an important transport mechanism. Estimated volatilization half-lives indicate that it will be non-volatile from surface water. Volatilization from dry surface is also not expected based on its vapor pressure. In the atmosphere, this compound is expected to exist solely in the particulate phase, based on its estimated vapor pressure. Particulates may be removed from air by wet or dry deposition.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	EPI; Professional judgment	Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. Cutoff value for non volatile compounds.
	Sediment/Soil Adsorption/ Desorption Coefficient – K_{oc}	>30,000 (Estimated)	EPI; EPA, 2011	Estimate based on a representative oligomer with a MW <1,000 that includes all monomers. Cutoff value for non mobile compounds according to SF assessment guidance.
	Level III Fugacity Model	Air = <1% (Estimated) Water = <1% Soil = 53% Sediment = 47%	EPI	Estimate based on a representative oligomer with a MW <1,000 that includes all monomers.
Persistence		**HIGH: The persistence for N-alkoxy hindered amine reaction products is based on an experimental guideline biodegradation study (4% removal after 28 days). Approximately 90% of the commercial N-alkoxy hindered amine reaction products substance has a MW >1,300 and is not anticipated to be assimilated by microorganisms. This polymer is not expected to be removed by other degradative processes under environmental conditions, such as hydrolysis, since it lacks the functional groups that hydrolyze under environmental conditions. This polymer does not contain chromophores that absorb at wavelengths >290 nm, and therefore it is not expected to be susceptible to direct photolysis by sunlight. The atmospheric half-life is estimated to be 19 minutes, although it is expected to exist primarily in the particulate phase in air.**		

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Water	**Aerobic Biodegradation**	Ready Test: Modified Sturm Test (OECD TG 301B); 4.37% biodegradation detected after 28 days in sewage sludge (Measured)	Toxicon, 1997	Adequate, guideline study.
	Volatilization Half-life for Model River	>1 year (Estimated)	EPI	
	Volatilization Half-life for Model Lake	>1 year (Estimated)	EPI	
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation	Not probable (Anaerobic-methanogenic biodegradation probability model)	EPI	Estimate based on a representative oligomer with a MW <1,000 that includes all monomers.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	19 minutes (Estimated)	EPI	Estimate based on a representative oligomer with a MW <1,000 that includes all monomers.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
	Hydrolysis	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to hydrolyze readily under environmental conditions.

N-alkoxy Hindered Amine Reaction Products CASRN 191680-81-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Environmental Half-Life		>180 days (Estimated)	EPI; PBT Profiler	Half-life estimated for the predominant compartment, as determined by EPI and the PBT Profiler methodology, for a representative oligomer with a MW <1000.
Bioaccumulation		**HIGH: A representative oligomer (with MW 770) that includes all combinations of monomers has an estimated BAF of 2,300; this BAF value, which accounts for metabolism, suggests that this substance has potential to bioaccumulate in higher trophic levels.**		
	Fish BCF	27 (Estimated)	EPI	Estimate based on a representative oligomer with a MW <1,000 that includes all monomers.
	BAF	2,300 (Estimated)	EPI	Estimate based on a representative oligomer with a MW <1,000 that includes all monomers.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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EPI *(EPIWIN/EPISUITE) Estimations Programs Interface for Windows*, Version 4.0. U.S. Environmental Protection Agency: Washington D.C. http://www.epa.gov/opptintr/exposure/.

ESIS (European chemical Substances Information System) Classification, labeling and packaging of dangerous substances annex VI to Regulation (EC) No 1272/2008 [Online] http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=cla (accessed on May 10, **2011**).

NICNAS. NA/999. National Industrial Chemicals Notification and Assessment Scheme. *1,3-Propanediamine, N,N''-1,2-ethanediylbis-, reaction products with cyclohexane and peroxidized N-butyl-2,2,6,6-tetramethyl-4-piperidinamine-2,4,6-trichloro-1,3,5-triazine reaction products (Flamestab NOR 116FF/TKA 45009).* File No. NA/869. **2001.**

PBT Profiler *Persistent (P),Bioaccumulative (B), and Toxic (T) Chemical (PBT)Profiler*, U.S. Environmental Protection Agency: Washington D.C. www.pbtprofiler.net.

Toxicon. TKA *45009: "Ready" Biodegradability: Carbon Dioxide Evolution Test (Modified Sturm Test)*; Toxicon Project J9703009e; Toxicon Environmental Sciences, 106 Coastal Way, Jupiter, Florida US. **1997.**

Phosphonate Oligomer

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

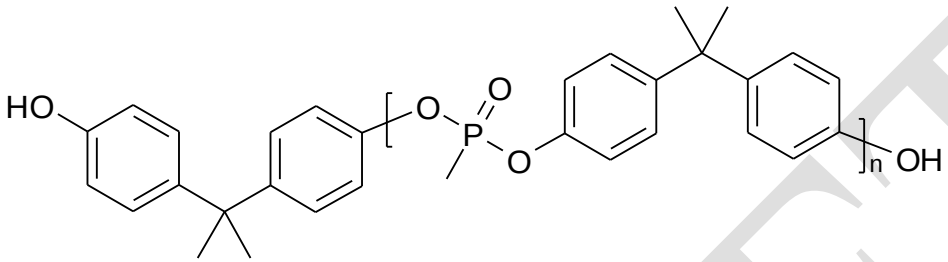
[§] Based on analogy to experimental data for a structurally similar compound.

[‡] The highest hazard designation of any of the oligomers with MW <1,000.

[¥] Phosphonate Oligomer, with a MW range of 1,000 to 5,000, may contain significant amounts of an impurity, depending on the final product preparation. This impurity has hazard designations that differ from the polymeric flame retardant, as follows: MODERATE-Experimental concern for repeated dose, skin sensitization and eye irritation; and HIGH-Experimental concern for reproductive, developmental, acute aquatic toxicity.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Phosphonate Oligomer	68664-06-2	L	*M*	*L*[§]	*L*[¥]	*L*[¥]	*M*[‡]	*L*[§¥]	*L*[§¥]		*M*[‡¥]	*M*[‡]	L[¥]	*H*[‡]	*VH*	*H*[‡]

Phosphonate Oligomer



Representative Structure

CASRN: 68664-06-2

MW: 1,000-5,000; 25% MW <1,000

MF: $C_{15}H_{16}O_2(C_{16}H_{17}O_3P)_n$
$C_{31}H_{33}O_5P$ (n =1);
$C_{47}H_{50}O_8P_2$ (n =2)

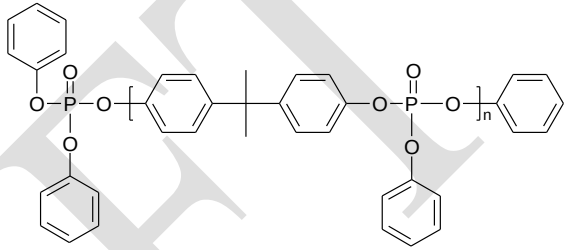
Physical Forms: Solid

Use: Flame retardant

SMILES: The polymer component with MW >1,000 components are not amenable to SMILES notation.
Phosphonate Oligomer: c1(O)ccc(C(C)(C)c2ccc(OP(C)(=O)Oc3ccccc3)cc2)cc1 (n=0; MW = 382);
c1(O)ccc(C(C)(C)c2ccc(OP(C)(=O)Oc3ccc(C(C)(C)c4ccc(O)cc4)cc3)cc2)cc1 (representative structure for n = 1; MW = 516);
c1(O)ccc(C(C)(C)c2ccc(OP(C)(=O)Oc3ccc(C(C)(C)c4ccc(OP(C)(=O)Oc5ccc(C(C)(C)c6ccc(O)cc6)cc5)cc4)cc3)cc2)cc1 (representative structure for n = 2, MW = 805); impurity: confidential SMILES.

Synonyms: FRX Oligomers (phosphonate oligomers), Phosphonic acid, P-methyl-, diphenyl ester, polymer with 4,4'-(1-methylethylidene)bis[phenol] (not a copolymer)

Chemical Considerations: This alternative is a polymer consisting of a large portion of higher (>1,000) MW oligomers and a smaller portion of lower (<1,000) MW oligomers. The higher MW oligomers, with a MW >1,000, are assessed together using the Sustainable Futures (SF) polymer assessment criteria in this report (EPA, 2010b). The n=1 and n=2 oligomers are those with a MW <1,000 and are assessed with EPI v4.1 due to an absence of experimental physical/chemical, environmental fate and aquatic toxicity values. Multiple n=1 and n=2 oligomer structures are possible from various starting material combinations. A representative structure was selected for determining the estimated n=1 and n=2 values, as identified in the SMILES section above. The human health designations for the lower MW oligomers are a result of identified structural alerts and experimental data from analogous compounds. Additionally, a confidential impurity may be present in polymer. The overall hazard designation for each endpoint represents the most conservative value of the higher MW oligomers and lower MW oligomers. A summary of the hazards of the confidential impurity is provided in hazard summary table as a footnote (♦).

<table>
<tr><td colspan="2">Polymeric: Yes
Oligomers: The polymers are produced from the trans-esterification of methyldiphenylphosphonate and bisphenol A. The MW of Phosphonate Oligomer ranges between 1,000 and 5,000. Oligomers with MW <1,000 are expected to be present in 25% of the Phosphonate Oligomer formulation.</td></tr>
<tr><td colspan="2">Metabolites, Degradates and Transformation Products: None</td></tr>
<tr><td>Analog: BAPP (181028-79-5)
Endpoint(s) using analog values: Genotoxicity; Skin Sensitization; Repeated Dose</td><td>Analog Structure:
 
BAPP (181028-79-5)</td></tr>
<tr><td colspan="2">Structural Alerts: Phenols, neurotoxicity (U.S. EPA, 2010a).</td></tr>
<tr><td colspan="2">Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).</td></tr>
<tr><td colspan="2">Hazard and Risk Assessments: None identified.</td></tr>
<tr><td colspan="2">U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.</td></tr>
</table>

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	90 softening point (Measured)	FRX MSDS, 2009	The value corresponds to a softening point for the polymer.
Boiling Point (°C)	>300 (Estimated for n ≥3 oligomers)	Professional judgment	Cutoff value used for large, high MW solid.
	>300 (Estimated for n=1; n=2 oligomers)	EPI; EPA, 1999	Cutoff value for high boiling point compounds according to HPV assessment guidance.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated for n ≥3 oligomers)	Professional judgment; EPA, 2010b	Cutoff value for large, high MW polymers according to SF polymer assessment guidance.
	$<10^{-8}$ (Estimated for n=1; n=2 oligomers)	EPI; EPA, 2011	Cutoff value for nonvolatile compounds according to SF assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated for n ≥3 oligomers)	Professional judgment; EPA, 2010b	Cutoff value for large, high MW non-ionic polymers according to SF polymer assessment guidance.
	0.0015 (Estimated for n=1)	EPI	
	$<10^{-3}$ (Estimated for n=2)	EPI; EPA, 1999	Cutoff value for non soluble compounds according to HPV assessment guidance.
Log K_{ow}	Estimated for n ≥3 oligomers	Professional judgment	This polymer is not amenable to available estimation methods.
	7.2 (Estimated for n=1)	EPI	
	>10 (Estimated for n=2)	EPI; EPA, 2011	Cutoff value used according to SF assessment guidance.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.

Phosphonate Oligomer CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Explosivity		Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis				No data located.
pH		Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a		Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**No absorption is expected for any route of exposure for the neat material of Phosphonate Oligomer. The lower MW fraction, in solution, is predicted to have poor absorption for all routes. The higher MW oligomers are large, with a MW >1,000. Based on professional judgment, Phosphonate Oligomer is expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No absorption of Phosphonate Oligomer is expected for any route; poor absorption of the low MW fraction when in solution is expected for all routes. (Estimated)	Professional judgment	Estimated based on physical/chemical properties and limited bioavailability.
Acute Mammalian Toxicity		**LOW: The majority of this polymer consists of high MW oligomers. Based on experimental LD_{50} values of >2,000 mg/kg. This compound is also expected to have limited bioavailability and therefore is of low potential for acute mammalian toxicity.**		
	Oral	Rat oral LD_{50} > 2,000 mg/kg	FRX Polymers, Inc., 2010	Conducted according to OECD 420; test substance: FRX oligophosphonate.
	Dermal	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
	Inhalation			
Carcinogenicity		**MODERATE: There is uncertainty for Phosphonate Oligomer due to the lack of data for this substance. Carcinogenic effects cannot be ruled out.**		

Phosphonate Oligomer CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	OncoLogic Results			This polymer is not amenable to available estimation methods.
	Carcinogenicity (Rat and Mouse)			No data located.
	Combined Chronic Toxicity/ Carcinogenicity			No data located.
Genotoxicity		**LOW: Estimated for Phosphonate Oligomer based on analogy to BAPP (181028-79-5).**		
	Gene Mutation *in vitro*	Limited bioavailability expected for the high MW (>1,000) components. (Estimated)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
		Negative, Ames assay (standard plate) in *Salmonella typhimurium* strains TA98, TA100, TA1537, TA1535, and *E. coli* WP2uvrA with and without metabolic activation. (Estimated by analogy)	NICNAS NA/869, 2000; Professional judgment	Based on analogy to BAPP; Sufficient study details were reported in a secondary source; used OECD test guidelines (OECD 471 & 472). Data are for commercial mixture.
		Negative, Ames assay (standard plate) in *Salmonella typhimurium* strains TA98, TA100, TA1537, TA1535, and *E. coli* WP2uvrA with and without metabolic activation (Estimated by analogy)	NICNAS NA/773, 2000; Professional judgment	Based on analogy to BAPP. Sufficient study details were reported in a secondary source; used OECD test guidelines (OECD 471 & 472). Data are for the predominant component.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	Negative for chromosome aberrations in CHL/IU cells with and without metabolic activation.	FRX Polymers, Inc, 2011c	Conducted in compliance with GLP.
		Negative, did not produce chromosomal aberrations in CHO cells with and without metabolic activation. (Estimated by analogy)	NICNAS NA/869, 2000; Professional judgment	Based on analogy to BAPP. Sufficient study details were reported in a secondary source; used OECD test guidelines (OECD 473). Data are for commercial mixture.

Phosphonate Oligomer CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Negative, did not produce chromosomal aberrations in CHL cells with and without metabolic activation. (Estimated by analogy)	NICNAS NA/773, 2000; Professional judgment	Based on analogy to BAPP. Sufficient study details were reported in a secondary source; used EC/EEC test guidelines (EC Directives 87/18/EEC and 88/320/EEC). Data are for the predominant component.
	Chromosomal Aberrations *in vivo*	Negative; did not increase micronucleated polychromatic erythrocytes in bone marrow cells of mice. (Estimated by analogy)	NICNAS NA/869, 2000; Professional judgment	Based on analogy to BAPP. Sufficient study details were reported in a secondary source; used OECD test guidelines (OECD 474). Data are for commercial mixture.
	DNA Damage and Repair			No data located.
	Other			
Reproductive Effects		**LOW: The high MW components of Phosphonate Oligomer are expected to have limited bioavailability and therefore have low potential for reproductive effects based on professional judgment and the SF polymer assessment guidance. No structural alerts or mechanistic pathways associated with reproductive effects were identified for the lower MW oligomeric material (n=1 and n=2).**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected. (Estimated for n ≥3 oligomers)	Professional judgment**;** EPA, 2010b	Based on SF polymer assessment guidance.
		For n=1 and n=2 oligomers	Professional judgment	No structural alerts or mechanistic pathways associated with reproductive effects were identified for the lower MW oligomeric material.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected. (Estimated for n≥3 oligomers)	Professional judgment**;** EPA, 2010b	Based on SF polymer assessment guidance.
		For n=1 and n=2 oligomers	Professional judgment	No structural alerts or mechanistic pathways associated with reproductive effects were identified for the lower MW oligomeric material.

Phosphonate Oligomer CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Reproduction and Fertility Effects	Limited bioavailability expected. (Estimated for n ≥3 oligomers)	Professional judgment**;** EPA, 2010b	Based on SF polymer assessment guidance.
		For n=1 and n=2 oligomers	Professional judgment	No structural alerts or mechanistic pathways associated with reproductive effects were identified for the lower MW oligomeric material.
Developmental Effects		**LOW: The high MW polymeric material is expected to have limited bioavailability and therefore has low potential for developmental effects based on professional judgment and the SF polymer assessment guidance. No structural alerts or mechanistic pathways associated with developmental effects were identified for the lower MW oligomeric material (n=1 and n=2).**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected. (Estimated for n≥3 oligomers)	Professional judgment**;** EPA, 2010b	Based on SF polymer assessment guidance.
		(Estimated for n=1 and n=2 oligomers)	Professional judgment	No structural alerts or mechanistic pathways associated with reproductive effects were identified for the lower MW oligomeric material.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected. (Estimated for n≥3 oligomers)	Professional judgment**;** EPA, 2010b	Based on SF polymer assessment guidance.
		(Estimated for n=1 and n=2 oligomers)	Professional judgment	No structural alerts or mechanistic pathways associated with reproductive effects were identified for the lower MW oligomeric material.
Neurotoxicity		**MODERATE: A moderate hazard is estimated for the Phosphonate Oligomer. There is potential for neurotoxicity based on the presence of the phenol structural alert.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected. (Estimated for n≥3 oligomers)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
Repeated Dose Effects		**LOW: A low hazard is estimated for the lower MW oligomers of Phosphonate Oligomer based on analogy to BAPP (181028-79-5), which has a low concern for this endpoint. The hazard designation for n ≥ 3 is also of low hazard potential based on limited bioavailability.**		

Phosphonate Oligomer CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Limited bioavailability expected. (Estimated for n≥3 oligomers)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
		In a 28-day oral (gavage) study in Sprague-Dawley rats, there were no treatment-related changes in any of the parameters measured. NOEL ≥1,000 mg/kg-day (highest dose tested) (Estimated by analogy)	NICNAS NA/869, 2000; Professional judgment	Based on analogy to BAPP. Sufficient study details were reported; used OECD test guidelines (OECD 407). Data are for commercial mixture.
		In a 28-day oral (gavage) study in Sprague-Dawley rats, there were no treatment-related changes in any of the parameters measured NOEL ≥1,000 mg/kg-day (highest dose tested). (Estimated by analogy)	NICNAS NA/773, 2000; Professional judgment	Based on analogy to BAPP. Sufficient study details were reported; used EEC test guidelines (EEC Directive 92/69/EEC, Method B7). Data are for the predominant component.
Skin Sensitization		**LOW: Based on expert judgment, Phosphonate Oligomer is not estimated to have potential for skin sensitization. No experimental data was located for this compound. For the lower MW oligomers, the hazard designation is low based on analogy to BAPP (181028-79-5).**		
	Skin Sensitization	Not expected to be a skin sensitizer (Estimated for n≥3 oligomers)	Expert judgment	Estimated based on expert judgment.
		Non-sensitizing, guinea pig (Estimated by analogy)	NICNAS NA/869, 2000; Professional judgment	Based on analogy to BAPP. Conducted according to EEC/OECD guidelines (OECD 406). Data are for commercial mixture.
		Non-sensitizing, guinea pig (Estimated by analogy)	NICNAS NA/773, 2000; Professional judgment	Based on analogy to BAPP. Conducted according to EEC/OECD guidelines (OECD 406). Data are for the predominant component.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**MODERATE: There is uncertain potential for irritation for Phosphonate Oligomer based on the phenol moieties. No experimental data located for the polymer.**		

Phosphonate Oligomer CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Eye Irritation	Uncertain potential for irritation based on the phenol moieties. (Estimated)	Professional judgment	Estimated based on phenol moieties.
Dermal Irritation		**MODERATE: The potential for irritation for Phosphonate Oligomer is based on the phenol moieties structural alert.**		
	Dermal Irritation	Uncertain potential for irritation based on the phenol moieties. (Estimated)	Professional judgment	Estimated based on phenol moieties.
Endocrine Activity		**Based on expert judgment; Phosphonate Oligomer is not expected to have endocrine activity due to its poor bioavailability and inability to be readily metabolized in the body.**		
		Limited bioavailability expected. (Estimated)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
Immunotoxicity		**Based on expert judgment; Phosphonate Oligomer is expected to have limited bioavailability and therefore is of low concern.**		
	Immune System Effects	Limited bioavailability expected. (Estimated)	Professional judgment; EPA, 2010b	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable for n≥3 oligomers. Esters, Esters (phosphate) and Polyphenols for n=1 and n=2.		
Acute Toxicity		**LOW: Estimated data for Phosphonate Oligomer suggest no effects at saturation (NES) for the acute aquatic toxicity endpoints for the n=1 and n=2 oligomers and the non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are estimated to have no effects at saturation (NES). These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Bioavailability is limited because this chemical cannot be absorbed through membranes due to large size.**		
Fish LC_{50}		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
		Fish 96-hour LC_{50} = 0.063 mg/L (Estimated for n=1) ECOSAR class: Esters	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Fish 96-hour LC_{50} = 0.17 mg/L (Estimated for n=1) ECOSAR class: Esters(phosphate)	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Fish 96-hour LC_{50} = 0.022 mg/L (Estimated for n=1) ECOSAR class: Phenols, Poly	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 5.5; NES are predicted for these endpoints.
	Fish 96-hour LC_{50} = 0.009 mg/L (Estimated for n=1) ECOSAR class: Neutral organics	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Fish 96-hour LC_{50} = 0.00081 mg/L (Estimated for n=2) ECOSAR class: Esters	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Fish 96-hour LC_{50} = 0.015 mg/L (Estimated for n=2) ECOSAR class: Esters(phosphate)	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Fish 96-hour LC_{50} = 0.00026 mg/L (Estimated for n=2) ECOSAR class: Phenols, Poly	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.5; NES are predicted for these endpoints.

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Fish 96-hour LC_{50} = 0.0000087 mg/L (Estimated for n=2) ECOSAR class: Neutral organics	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Daphnid LC_{50}	*Daphnia magna* 48-hour EC_{50} > 0.275 mg/L; semi static conditions. (Experimental)	FRX Polymers, Inc, 2011a	Study conducted according to guidelines for daphnia acute immobilization test; test substance purity = 96.39%. It is not clear if the reported value represent nominal or actual concentrations of dissolved species.
	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
	Daphnid 48-hour LC_{50} = 0.075 mg/L (Estimated for n=1) ECOSAR class: Esters	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Daphnid 48-hour LC_{50} = 0.00021 mg/L (Estimated for n=1) ECOSAR class: Esters(phosphate)	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Daphnid 48-hour LC_{50} = 0.022 mg/L (Estimated for n=1) ECOSAR class: Phenols, Poly	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 5.5; NES are predicted for these endpoints.
	Daphnid 48-hour LC_{50} = 0.013 mg/L (Estimated for n=1) ECOSAR class: Neutral organics	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Daphnid 48-hour LC_{50} = 0.00066 mg/L (Estimated for n=2) ECOSAR class: Esters	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Daphnid 48-hour LC_{50} = 0.000015 mg/L (Estimated for n=2) ECOSAR class: Esters(phosphate)	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
	Daphnid 48-hour LC_{50} = 0.000061 mg/L (Estimated for n=2) ECOSAR class: Phenols, Poly	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.5; NES are predicted for these endpoints.
	Daphnid 48-hour LC_{50} = 0.000024 mg/L (Estimated for n=2) ECOSAR class: Neutral organics	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted for these endpoints.
Green Algae EC_{50}	*Pseudokirchneriella subcapitata* 72-hour EC_{50} > 0.124 mg/L	FRX Polymers, Inc, 2011b	Study conducted according to guidelines for algal growth inhibition test; test substance purity = 96.39%. It is not clear if the reported value represent nominal or actual concentrations of dissolved species.
	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Green algae 96-hour EC_{50} = 0.014 mg/L (Estimated for n=1) ECOSAR class: Esters	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
	Green algae 96-hour EC_{50} = 0.006 mg/L (Estimated for n=1) ECOSAR class: Esters(phosphate)	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
	Green algae 96-hour EC_{50} = 0.19 mg/L (Estimated for n=1) ECOSAR class: Phenols, Poly	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
	Green algae 96-hour EC_{50} = 0.012 mg/L (Estimated for n=1) ECOSAR class: Neutral organics	EPI	NES: The log K_{ow} of 7.2 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
	Green algae 96-hour EC_{50} = 0.000069 mg/L (Estimated for n=2) ECOSAR class: Esters	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
	Green algae 96-hour EC_{50} = 0.00000051 mg/L (Estimated for n=2) ECOSAR class: Esters(phosphate)	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Green algae 96-hour EC_{50} = 0.018 mg/L (Estimated for n=2) ECOSAR class: Phenols, Poly	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
	Green algae 96-hour EC_{50} = 0.000024 mg/L (Estimated for n=2) ECOSAR class: Neutral organics	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted for these endpoints.
Chronic Aquatic Toxicity	**HIGH: Based on estimated data for the acute aquatic toxicity endpoints for the n=1 and n=2 oligomers. It should be noted that the estimated values may be near the limit of the domain of applicability for this estimation model and there is a high degree of uncertainty in these estimated results.**		
Fish ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
	Fish 30-day ChV = 0.00158 mg/L (Estimated for n=1) ECOSAR class: Esters	EPI	The estimated value is close to the cutoff value of this ECOSAR class. There is a high degree of uncertainty as the estimates for this compound are at the limits of the domain for this estimation model.
	Fish 30-day ChV = 0.005 mg/L (Estimated for n=1) ECOSAR class: Esters(phosphate)	EPI	The estimated value is close to the cutoff value of this ECOSAR class. There is a high degree of uncertainty as the estimates for this compound are at the limits of the domain for this estimation model.

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Fish 30-day ChV = 0.005 mg/L (Estimated for n=1) ECOSAR class: Phenols, Poly	EPI	The estimated value is close to the cutoff value of this ECOSAR class. There is a high degree of uncertainty as the estimates for this compound are at the limits of the domain for this estimation model.
	Fish 30-day ChV = 0.0015 mg/L (Estimated for n=1) ECOSAR class: Neutral organics	EPI	The estimated value is close to the cutoff value of this ECOSAR class. There is a high degree of uncertainty as the estimates for this compound are at the limits of the domain for this estimation model.
	Fish 30-day ChV = 0.0000096 mg/L (Estimated for n=2) ECOSAR class: Esters	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
	Fish 30-day ChV = 0.003 mg/L (Estimated for n=2) ECOSAR class: Esters(phosphate)	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
	Fish 30-day ChV = 0.000037 mg/L (Estimated for n=2) ECOSAR class: Phenols, Poly	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
	Fish 30-day ChV = 0.0000022 mg/L (Estimated for n=2) ECOSAR class: Neutral organics	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Daphnid ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
	Daphnid Daphnid ChV = 0.011 mg/L (Estimated for n=1) ECOSAR class: Esters	EPI	The estimated value is close to the cutoff value of this ECOSAR class. There is a high degree of uncertainty as the estimates for this compound are at the limits of the domain for this estimation model.
	Daphnid Daphnid ChV = 0.006 mg/L (Estimated for n=1) ECOSAR class: Phenols, Poly	EPI	The estimated value is close to the cutoff value of this ECOSAR class. There is a high degree of uncertainty as the estimates for this compound are at the limits of the domain for this estimation model.
	Daphnid Daphnid ChV = 0.003 mg/L (Estimated for n=1) ECOSAR class: Neutral organics	EPI	The estimated value is close to the cutoff value of this ECOSAR class. There is a high degree of uncertainty as the estimates for this compound are at the limits of the domain for this estimation model.
	Daphnid Daphnid ChV = 0.000036 mg/L (Estimated for n=2) ECOSAR class: Esters	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Daphnid Daphnid ChV = 0.000013 mg/L (Estimated for n=2) ECOSAR class: Phenols, Poly	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
	Daphnid Daphnid ChV = 0.00001 mg/L (Estimated for n=2) ECOSAR class: Neutral organics	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
Green Algae ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
	Green algae ChV = 0.019 mg/L (Estimated for n=1) ECOSAR class: Esters	EPI	Chemical may not be soluble enough to measure this predicted effect; ChV value exceeds water solubility.
	Green algae ChV = 0.16 mg/L (Estimated for n=1) ECOSAR class: Esters(phosphate)	EPI	Chemical may not be soluble enough to measure this predicted effect; ChV value exceeds water solubility.
	Green algae ChV = 0.054 mg/L (Estimated for n=1) ECOSAR class: Phenols, Poly	EPI	Chemical may not be soluble enough to measure this predicted effect; ChV value exceeds water solubility.
	Green algae ChV = 0.034 mg/L (Estimated for n=1) ECOSAR class: Neutral organics	EPI	Chemical may not be soluble enough to measure this predicted effect; ChV value exceeds water solubility.

Phosphonate Oligomer CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Green algae ChV = 0.0003 mg/L (Estimated for n=2) ECOSAR class: Esters	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
		Green algae ChV = 0.0017 mg/L (Estimated for n=2) ECOSAR class: Esters(phosphate)	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
		Green algae ChV = 0.009 mg/L (Estimated for n=2) ECOSAR class: Phenols, Poly	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
		Green algae ChV = 0.00037 mg/L (Estimated for n=2) ECOSAR class: Neutral organics	EPI	NES: The log K_{ow} of 10.8 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted for these endpoints.
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that this polymer is anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of $<10^{-8}$ atm-m^3/mole indicates that it is not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that it is not anticipated to migrate from soil into groundwater and also has the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated for n ≥3 oligomers)	Professional judgment; EPA, 2010b	Cutoff value used for large, high MW polymers. High MW polymers are expected to have low vapor pressure and are not expected to undergo volatilization according to SF polymer assessment guidance.

Phosphonate Oligomer CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		$<10^{-8}$ (Estimated for the n=1 and n=2)	EPI; Professional judgment	Cutoff value for non volatile compounds.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated for n≥3 oligomers)	Professional judgment; EPA, 2010b	Cutoff value used for large, high MW polymers. High MW polymers are expected to adsorb strongly to soil and sediment according to SF polymer assessment guidance.
		>30,000 (Estimated for the n=1 and n=2)	EPI; EPA, 2011	Cutoff value for non mobile compounds according to SF assessment guidance.
	Level III Fugacity Model	Air ≤ 1% Water < 1% Soil = 53% Sediment = 46% (Estimated for n = 1 and n = 2)	EPI	No data located for the high MW component of the polymers.
Persistence		**VERY HIGH: The high MW components (MW >1000) of this polymer are expected to have negligible water solubility and poor bioavailability to microorganisms indicating that neither biodegradation nor hydrolysis are expected to be important removal processes in the environment. The polymer does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths. Evaluation of these degradation values suggest a half-life of >180 days.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated for n ≥3 oligomers)	Professional judgment; EPA, 2010b	High MW polymers are expected to be non-biodegradable according to SF polymer assessment guidance.
		Weeks (Primary Survey Model) Recalcitrant (Ultimate Survey Model) for n=1	EPI	
		Weeks-months (Primary Survey Model Recalcitrant (Ultimate Survey Model) for n=2	EPI	

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PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	This polymer is anticipated to be non volatile.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	This polymer is anticipated to be non volatile.
Soil	**Aerobic Biodegradation**	Recalcitrant (Estimated for n ≥3 oligomers)	Professional judgment; EPA, 2010b	High MW polymers are expected to be non-biodegradable according to SF polymer assessment guidance due to their limited bioavailability.
	Anaerobic Biodegradation	Recalcitrant (Estimated for n ≥3 oligomers)	Professional judgment; EPA, 2010b	High MW polymers are expected to be resistant to removal under anoxic conditions due to their limited bioavailability.
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Environmental Half-life	>180 days (Estimated)	Professional judgment	The majority of this substance has a MW >1,000 and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to be removed by other degradative processes under environmental conditions because of limited water solubility and limited partitioning to air.
Bioaccumulation	**HIGH: Although measured BCF values are available, estimated BAF values are incorporated for a conservative approach. The BAF estimate is consistent with the potential for bioaccumulation that is anticipated. The high MW oligomers do not contribute to the bioaccumulation designation. The high MW oligomers are expected to have poor bioavailability and are not expected to be bioaccumulative.**		

<table>
<tr><th colspan="4">Phosphonate Oligomer CASRN 68664-06-2</th></tr>
<tr><th colspan="2">PROPERTY/ENDPOINT</th><th>DATA</th><th>REFERENCE</th><th>DATA QUALITY</th></tr>
<tr><td></td><td>Fish BCF</td><td>Eight components of this polymer with MW <1,000 were tested according to “Bioconcentration test of chemical substances in fish and shellfish” in Cyprinus carpio. Test concentrations of 0.01 and 0.001 mg/L.
Results:
<table>
<tr><th>Mass to charge ratio (m/z)</th><th>High Conc. Level BCF</th><th>Low Conc. Level BCF</th></tr>
<tr><td>383</td><td>≤41</td><td><222</td></tr>
<tr><td>517</td><td>≤85</td><td><223-242</td></tr>
<tr><td>688</td><td>≤60</td><td><142</td></tr>
<tr><td>822</td><td>≤67</td><td><114-280</td></tr>
<tr><td>976</td><td>≤53</td><td><128</td></tr>
<tr><td>537</td><td>274</td><td><200-560</td></tr>
<tr><td>577</td><td>82-250</td><td><200-534</td></tr>
<tr><td>825</td><td><20-52</td><td><200</td></tr>
</table></td><td>FRX Polymers, 2012</td><td>Reported as Japanese notification, guideline study.</td></tr>
<tr><td></td><td></td><td><100 (Estimated for n≥3 oligomers)</td><td>Professional judgment</td><td>The substance has a MW >1,000 and is not anticipated to be taken up by aquatic organisms; therefore, bioconcentration is not expected.</td></tr>
<tr><td></td><td></td><td>10,000 (Estimated for n=1)</td><td>EPI</td><td></td></tr>
<tr><td></td><td></td><td>190 (Estimated for n=2)</td><td>EPI</td><td></td></tr>
<tr><td></td><td>BAF</td><td>For n ≥3 oligomers</td><td></td><td>No data located.</td></tr>
<tr><td></td><td></td><td>780,000 (Estimated for n=1)</td><td>EPI</td><td></td></tr>
<tr><td></td><td></td><td>64,000 (Estimated for n=2)</td><td>EPI</td><td></td></tr>
</table>

Phosphonate Oligomer CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING			
Environmental Monitoring	No data located.		
Ecological Biomonitoring	No data located.		
Human Biomonitoring	This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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NICNAS NA/869. National Industrial Chemicals Notification and Assessment Scheme. *Phosphoric Trichloride, Reaction Products with Bisphenol A and Phenol)*. File No. NA/869. **2000**.

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Polyphosphonate

Screening Level Hazard Summary

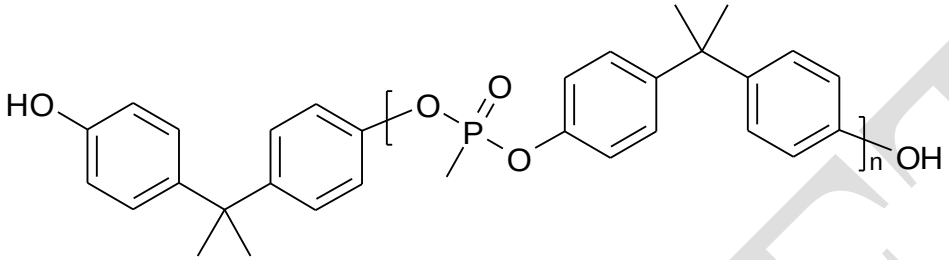
This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

[d] This hazard designation is driven by potential for lung overloading as a result of dust forming operations.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Polyphosphonate	68664-06-2	L	*L*	*L*	*L*	*L*	*L*	*M*[d]	*L*		*L*	*L*	*L*	*L*	*VH*	*L*

Polyphosphonate



Representative Structure

CASRN: 68664-06-2

MW: 10,000 to 50,000;
<1% MW <1,000

MF: $C_{15}H_{16}O_2(C_{16}H_{17}O_3P)_n$

Physical Forms: Solid

Use: Flame retardant

SMILES: The polymer components with MW >1,000 are not amenable to SMILES notation.

Synonyms: FRX 100 (polyphosphonate) (Polymeric additive); FRX100; Phosphonic acid, P-methyl-, diphenyl ester, polymer with 4,4'-(1-methylethylidene)bis[phenol]

Chemical Considerations: This alternative is a high MW polymer with <1% low (<1,000) MW oligomers. The high MW oligomers, with a MW >1,000, are assessed together using the Sustainable Futures (SF) polymer assessment criteria in this report (U.S. EPA, 2010).

Polymeric: Yes
Oligomers: The polymer is produced from the condensation of methyldiphenylphosphonate and bisphenol A equivalents. The MW of polyphosphonate ranges between 10,000 and 50,000. Oligomers with MW <1,000 are expected to be present at <1% in the polyphosphonate mixture.

Metabolites, Degradates and Transformation Products: None

Analog: No analog **Endpoint(s) using analog values:** Not applicable	**Analog Structure:** Not applicable

Structural Alerts: No data located.

Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).

Hazard and Risk Assessments: None identified.

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.

Polyphosphonate CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	90 softening point (Measured)	FRX MSDS, 2009	The value corresponds to a softening point for the polymer.
Boiling Point (°C)	>300 (Estimated)	Professional judgment	Cutoff value used for large, high MW solid.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW polymers according to SF polymer assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW non-ionic polymers according to SF polymer assessment guidance.
Log K_{ow}			No data located; polymers with a MW >1,000 are outside the domain of the available estimation methods.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.

Polyphosphonate CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**No absorption is expected for any route of exposure for polyphosphonate. This polymer is large, with a MW >1,000. Based on professional judgment, it is expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No absorption is expected for any route of exposure (Estimated)	Professional judgment	Estimated based on professional judgment.
Acute Mammalian Toxicity		**LOW: Based on experimental LD_{50} values > 2,000 mg/kg. This compound is also expected to have limited bioavailability and therefore is of low potential for acute mammalian toxicity.**		
	Oral	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
		Rat oral LD_{50} > 2,000 mg/kg	FRX Polymers, Inc., 2011	Conducted according to OECD 420; test substance: FRX polyphosphonate.
	Dermal			No data located.
	Inhalation			No data located.
Carcinogenicity		**LOW: This polymer is large, with a MW >1,000. Based on professional judgment, it is expected to have few to no residual monomers. Additionally, crosslinking, swellability, dispersability, reactive functional groups, inhalation potential, and hindered amine groups are not expected. Therefore, there is low potential for carcinogenicity.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)	Limited bioavailability expected; crosslinking swellability, dispersability, reactive functional groups, inhalation potential, and hindered amine groups are not expected. (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Combined Chronic Toxicity/ Carcinogenicity			

Polyphosphonate CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Genotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for genotoxicity.**		
	Gene Mutation *in vitro*	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Gene Mutation *in vivo*			
	Chromosomal Aberrations *in vitro*			
	Chromosomal Aberrations *in vivo*			
	DNA Damage and Repair			
	Other (Mitotic Gene Conversion)			
Reproductive Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for reproductive effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			
Developmental Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for developmental effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			

Polyphosphonate CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Postnatal Development			
Neurotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for neurotoxicity.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
Repeated Dose Effects		**MODERATE: This polymer is large, with a MW >1,000. Based on professional judgment, it is expected to have limited bioavailability. However, because the MW of polyphosphonate is >10,000 there is the possibility of lung overloading in dust forming conditions if the compound is insoluble in water.**		
		Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
		This polymer's MW_n is >10,000; potential for irreversible lung damage as a result of lung overloading. (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
Skin Sensitization		**LOW: Based on expert judgment, polyphosphonate is estimated not to have potential for skin sensitization**		
	Skin Sensitization	Not expected to be a skin sensitizer (Estimated)	Expert judgment	Estimated based on expert judgment by analogy to other high MW polymers with similar structural features.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Based on expert judgment, polyphosphonate is estimated to not have potential for eye irritation.**		
	Eye Irritation	Not expected to be an eye irritant (Estimated)	Expert judgment	Estimated based on expert judgment by analogy to other high MW polymers with similar structural features.
Dermal Irritation		**LOW: Based on expert judgment, polyphosphonate is estimated to not have potential for dermal irritation.**		
	Dermal Irritation	Not expected to be a skin irritant (Estimated)	Expert judgment	Estimated based on expert judgment by analogy to other high MW polymers with similar structural features.

Polyphosphonate CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Endocrine Activity		**No data located. This polymer is large, with a MW >1,000. Based on professional judgment, polyphosphonate is not expected to have endocrine activity due to its poor bioavailability and inability to be readily metabolized in the body.**		
		Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
Immunotoxicity		**Based on professional judgment polyphosphonate is expected to have limited bioavailability and therefore is of low concern.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**LOW: Non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to have no effects at saturation (NES). These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Bioavailability is limited because this chemical cannot be absorbed through membranes due to its large size.**		
Fish LC_{50}		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity		**LOW: Non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to display NES. These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Bioavailability is limited because this chemical cannot be absorbed through membranes due to its large size.**		

Polyphosphonate CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Fish ChV		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid ChV		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae ChV		NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that this polymer is anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of $<10^{-8}$ atm-m^3/mole indicates that it is not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that it is not anticipated to migrate from soil into groundwater and also has the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value used for large, high MW polymers. High MW polymers are expected to have low vapor pressure and are not expected to undergo volatilization according to SF polymer assessment guidance.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; EPA, 2010	Cutoff value used for large, high MW polymers. High MW polymers are expected to adsorb strongly to soil and sediment according to SF polymer assessment guidance.

Polyphosphonate CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Level III Fugacity Model			No data located.
Persistence		**VERY HIGH: This polymer is large, with a MW >1,000. It is expected to have negligible water solubility and poor bioavailability to microorganisms indicating that neither biodegradation nor hydrolysis are expected to be important removal processes in the environment. The polymer does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths. Evaluation of these degradation values suggest a half-life of >180 days.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to be non-biodegradable according to SF polymer assessment guidance.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	This high MW polymer is anticipated to be non volatile.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	This high MW polymer is anticipated to be non volatile.
Soil	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to be non-biodegradable according to SF polymer assessment guidance due to their limited bioavailability.
	Anaerobic Biodegradation	Recalcitrant (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to be resistant to removal under anoxic conditions due to their limited bioavailability.
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.

Polyphosphonate CASRN 68664-06-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.
Environmental Half-life		>180 days (Estimated)	Professional Judgment	The majority of this substance has a MW >1,000 and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to be removed by other degradative processes under environmental conditions because of limited water solubility and limited partitioning to air.
Bioaccumulation		**LOW: This polymer is large, with a MW >1,000. It is expected to have poor bioavailability indicating that this polymer should be of low potential for bioaccumulation.**		
	Fish BCF	<100 (Estimated)	Professional judgment	The majority of this substance has a MW >1,000 and is not anticipated to be taken up by aquatic organisms; therefore, bioconcentration is not expected.
	BAF			No data located.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		

Polyphosphonate CASRN 68664-06-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Ecological Biomonitoring	No data located.		
Human Biomonitoring	This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

Boethling, R., Mackay, D. *Handbook of Property Estimation Methods for Chemicals, Environmental Health Sciences*. Boca Raton: Lewis Publishers. **2000**.

Centers for Disease Control and Prevention (CDC). *Fourth National Report on Human Exposure to Environmental Chemicals, Updated Tables.* Department of Health and Human Services **2011.** Available at: http://www.cdc.gov/exposurereport/ as of May 10, 2011

[SF Polymer Assessment Guidance] Environmental Protection Agency (EPA). Sustainable Futures Summary Assessment. *Interpretive Assistance Document for Assessment of Polymers.* U.S. Environmental Protection Agency: Washington D.C. **2010**. http://www.epa.gov/oppt/sf/pubs/iad_polymers_042010.pdf as of September 2, 2011.

European chemical Substances Information System (ESIS) Classification, Labeling and Packaging of Dangerous Substances Annex VI to Regulation (EC) No 1272/2008 [Online] available at: http://esis.jrc.ec.europa.eu/home.php as of May 10, **2011**.

FRX Polymers. *FRX 100 Homopolymer Material Safety Data Sheet (MSDS)*. Revised October 2, **2009**.

FRX Polymers, Inc. FRX polyphosphonate: Acute oral toxicity in the rat – fixed dose method. FRX Polymers, Inc. Chelmsford, MA. Project number 3224/0001. **2011**. (Submitted unpublished study).

Poly[phosphonate-co-carbonate]

Screening Level Hazard Summary

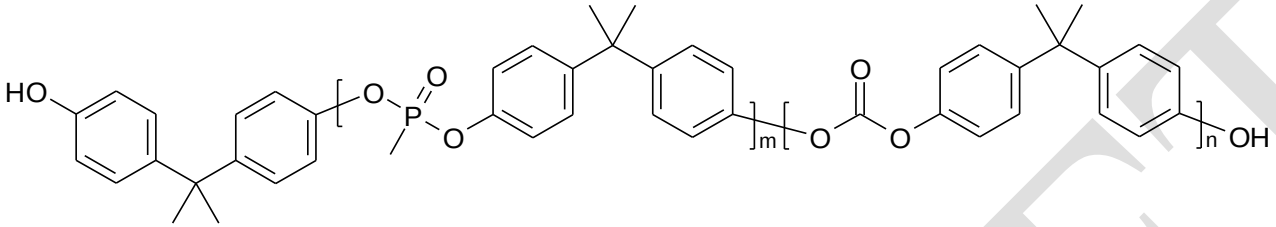
This table only contains information regarding the inherent hazards of flame-retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

[d] This hazard designation is driven by potential for lung overloading as a result of dust forming operations.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environ-mental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Poly[phosphonate-co-carbonate]	77226-90-5	L	*L*	*L*	*L*	*L*	*L*	*M*[d]	*L*		*L*	*L*	*L*	*L*	*VH*	*L*

Poly[phosphonate-co-carbonate]



Representative structure

CASRN: 77226-90-5

MW: >1,000; <1% <1,000

MF: $C_{15}H_{16}O_2(C_{16}H_{14}O_3)_n(C_{16}H_{17}O_3P)_m$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: This polymer with MW >1,000 and <1% low MW components is not amenable to SMILES notation.

Synonyms: Carbonic acid, diphenyl ester, polymer with diphenyl P-methylphosphonate and 4,4'- (1-methylethylidene)bis[phenol]; FRX CO35; FRX CO60

Chemical Considerations: This alternative is a polymer. Poly[phosphonate-co-carbonate] polymers differ in their ratio of polyphosphonate/polycarbonate (m to n) but would have identical hazard characterizations. The MW of the oligomers are generally >1,000 and are assessed together using the Sustainable Futures (SF) polymer assessment criteria (U.S. EPA, 2010). Representative structure drawn to show simplest combination of all feedstocks.

Polymeric: Yes
Oligomers: The MW for the Poly[phosphonate-co-carbonate] polymers range between 10,000 and 50,000; with <1% MW <1,000 oligomers expected.

Metabolites, Degradates and Transformation Products: None

Analog: No analog
Endpoint(s) using analog values: Not applicable

Analog Structure: Not applicable

Structural Alerts: None identified

Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011)

Hazard and Risk Assessments: None identified

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory and is a commenced Premanufacture Notice substance. This chemical is exempt from reporting under the Inventory Update Rule.

Poly[phosphonate-co-carbonate] CASRN 77226-90-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	220–250 (glass transition temperature) (Measured)	FRX MSDS, 2009	The melting points reported cover a broad range and are anticipated to be the formulation specific liquid-glass transition temperature or softening point.
	120 (softening point) (Measured)	FRX MSDS, 2009	
Boiling Point (°C)	>300 (Estimated)	Professional judgment	Cutoff value used for large, high MW solid.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW polymers according to polymer assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	Professional judgment, EPA, 2010	Cutoff value for large, high MW non-ionic polymers according to polymer assessment guidance.
	Insoluble (Measured)	FRX MSDS, 2009	Nonspecific value provided by commercial supplier.
Log K_{ow}			No data located.
Flammability (Flash Point)	>450°C (Measured)	FRX MSDS, 2009	Sufficient details were not available to assess the quality of this study.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.

Poly[phosphonate-co-carbonate] CASRN 77226-90-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**There is no absorption expected for any route of exposure for the neat material. Poor absorption of the low MW fraction in solution can be expected for all routes. This polymer is large, with a MW >1,000. Based on professional judgment, it is expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No absorption of the neat material is expected for any route of exposure; poor absorption of low MW fraction in solution for all routes. (Estimated)	Professional judgment	Estimated based on physical/chemical properties and limited bioavailability.
Acute Mammalian Toxicity		**LOW: Based on experimental LD_{50} values > 2,000 mg/kg. This compound is also expected to have limited bioavailability and therefore is of low potential for acute mammalian toxicity.**		
Acute Lethality	**Oral**	Rat oral LD_{50} > 2,000 mg/kg	FRX Polymers, Inc., 2011	Conducted according to OECD 420; test substance: FRX polyphosphonate.
	Dermal	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Inhalation			
Carcinogenicity		**LOW: This polymer is large, with a MW >1,000. Based on expert judgment, it is expected to have few to no residual monomers. Additionally, crosslinking, swellability, dispersability, reactive functional groups, inhalation potential, and hindered amine groups are not expected. Therefore, there is low potential for carcinogenicity based on professional judgment and the SF polymer assessment guidance. No data located.**		
	OncoLogic Results	Limited bioavailability expected; crosslinking swellability, dispersability, reactive functional groups, inhalation potential, and hindered amine groups are not expected. (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Carcinogenicity (Rat and Mouse)			
	Combined Chronic Toxicity/ Carcinogenicity			

Poly[phosphonate-co-carbonate] CASRN 77226-90-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Genotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for genotoxicity.**		
	Gene Mutation *in vitro*	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Gene Mutation *in vivo*			
	Chromosomal Aberrations *in vitro*			
	Chromosomal Aberrations *in vivo*			
	DNA Damage and Repair			
	Other (Mitotic Gene Conversion)			
Reproductive Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for reproductive effects based on professional judgment.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			

Poly[phosphonate-co-carbonate] CASRN 77226-90-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for reproductive effects based on professional judgment.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			
	Postnatal Development			
Neurotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for neurotoxicity based on professional judgment.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
Repeated Dose Effects		**MODERATE: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability. However, because the MW is >10,000 there is the possibility of lung overloading in dust forming conditions if the compound is insoluble in water. Based on professional judgment.**		
		This polymer's MW_n is >10,000; potential for irreversible lung damage as a result of lung overloading (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
Skin Sensitization		**LOW: Estimated to not have potential for skin sensitization based on expert judgment. No data located.**		
	Skin Sensitization	Not expected to be a skin sensitizer (Estimated)	Expert judgment	Estimated based on expert judgment.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.

Poly[phosphonate-co-carbonate] CASRN 77226-90-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Eye Irritation		**LOW: Uncertain potential for irritation based on the phenol moieties and professional judgment. No data located.**		
	Eye Irritation	Uncertain potential for irritation based on the phenol moieties. (Estimated)	Professional judgment	Estimated based on phenol moieties.
Dermal Irritation		**LOW: Uncertain potential for irritation based on the phenol moieties and professional judgment. No data located.**		
	Dermal Irritation	Uncertain potential for irritation based on the phenol moieties. (Estimated)	Professional judgment	Estimated based on phenol moieties.
Endocrine Activity		**No data located. This polymer is large, with a MW >1,000. Based on expert judgment, it is not expected to have endocrine activity due to its poor bioavailability and inability to be readily metabolized in the body.**		
		Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
Immunotoxicity		**This polymer is large, with a MW >1,000. Based on expert judgment, it is expected to have limited bioavailability and therefore is of low concern.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		

Poly[phosphonate-co-carbonate] CASRN 77226-90-5			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Acute Toxicity	**LOW: Non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to display no effects at saturation (NES). These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Bioavailability is limited because this chemical cannot be absorbed through membranes due to large size.**		
Fish LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity	**LOW: Non-ionic polymers with a MW >1,000 that do not contain reactive functional groups and are comprised of minimal low MW oligomers are estimated to display NES. These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low concern for those materials that display NES.**		
Fish ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will NES.
Daphnid ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Saltwater Invertebrate ChV			No data located.
Green Algae ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.

Poly[phosphonate-co-carbonate] CASRN 77226-90-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that these polymers are anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of $<10^{-8}$ atm-m^3/mole indicates that these are not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that they are not anticipated to migrate from soil into groundwater and have the potential to adsorb to sediment.**		
	Henry's Law Constant(atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to have low vapor pressure and are not expected to undergo volatilization according to polymer assessment guidance.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment	High MW polymers are expected to adsorb strongly to soil and sediment according to polymer assessment guidance.
	Level III Fugacity Model			No data located.
Persistence		**VERY HIGH: A very limited fraction of these polymers is expected to have a MW of <1,000; therefore, they are not anticipated to be assimilated by microorganisms and biodegradation is not expected to be an important removal process. They are also not expected to be removed by other degradative processes under environmental conditions because of limited water solubility and limited partitioning to air. They are expected to partition primarily to sediment and soil, where their estimated half-life is >1 year. The polymers lack the functional groups that hydrolyze under environmental conditions. These polymers do not contain chromophores that absorb at wavelengths >290 nm, and therefore, they are not expected to be susceptible to direct photolysis by sunlight.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment	Most high MW polymers are expected to be non-biodegradable according to polymer assessment guidance due to their limited bioavailability.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	This high MW polymer is anticipated to be non volatile.

Poly[phosphonate-co-carbonate] CASRN 77226-90-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	This high MW polymer is anticipated to be non volatile.
Soil	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment	High MW polymers are expected to be non-biodegradable according to polymer assessment guidance due to their limited bioavailability.
	Anaerobic Biodegradation	Recalcitrant (Estimated)	Professional judgment	High MW polymers are expected to be resistant to removal under anoxic conditions due to their limited bioavailability.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.

Poly[phosphonate-co-carbonate] CASRN 77226-90-5				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Environmental Half-Life		>180 days (Estimated)	Professional judgment	The substance has a MW >1,000 and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to be removed by other degradative processes under environmental conditions because of limited water solubility and limited partitioning to air.
Bioaccumulation		**LOW: These polymers are expected to have negligible water solubility and poor bioavailability indicating that these polymers should be of low potential for bioaccumulation.**		
	Fish BCF	<100 (Estimated)	Professional judgment	The substance has a MW >1,000 and is not anticipated to be assimilated by aquatic organisms; therefore, bioconcentration is not expected.
	BAF			No data located.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

Boethling, R., Mackay, D. *Handbook of Property Estimation Methods for Chemicals, Environmental Health Sciences*. Boca Raton: Lewis Publishers. **2000**.

Centers for Disease Control and Prevention (CDC). *Fourth National Report on Human Exposure to Environmental Chemicals, Updated Tables.* Department of Health and Human Services **2011.** Available at: http://www.cdc.gov/exposurereport/ as of May 10, 2011

European chemical Substances Information System (ESIS) Classification, Labeling and Packaging of Dangerous Substances Annex VI to Regulation (EC) No 1272/2008 [Online] available at: http://esis.jrc.ec.europa.eu/home.php as of May 10, 2011.

FRX MSDS, 2009. Material Safety Data Sheet. *FRX CO 35 Polyphosphonate Copolymer (CAS 77226-90-5)*. Chelmsford, MA. **2009.**

FRX Polymers, Inc. FRX polyphosphonate: Acute oral toxicity in the rat – fixed dose method. FRX Polymers, Inc. Chelmsford, MA. Project number 41103591. **2011**. (Submitted unpublished study).

[SF Polymer Assessment Guidance] Environmental Protection Agency (EPA). Sustainable Futures Summary Assessment. *Interpretive Assistance Document for Assessment of Polymers.* U.S. Environmental Protection Agency: Washington D.C. 2010. http://www.epa.gov/oppt/sf/pubs/iad_polymers_042010.pdf as of September 2, 2011.

Red Phosphorus

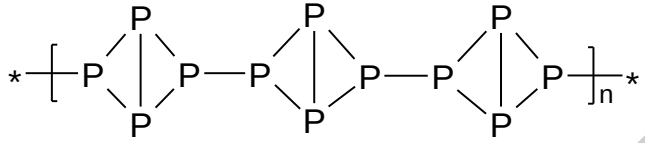
Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with a substance, including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from estimation software and professional judgment.

		Human Health Effects											Aquatic Toxicity		Environmental Fate	
Chemical	CASRN	Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Red Phosphorus	7723-14-0	VH	*L*	*M*	*L*	*L*	*L*	*L*	L		M	H	L	L	H	*L*

Red Phosphorus



CASRN: 7723-14-0

MW: >1,000 (Estimated)

MF: $(P_4)_n$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: This polymeric form of elemental phosphorous is not amenable to SMILES notation.

Synonyms: Phosphorus (TSCA Inventory), Red amorphous phosphorus, violet phosphorus, Exolit RP 605, Exolit RP 650, Exolit RP 652, Exolit RP 654, Hishigado, Hishigado AP, Hishigado CP, Hishigado NP 10, Hishigado PL, Hostaflam RP 602, Hostaflam RP 614, Hostaflam RP 622, Hostaflam RP 654, Novared 120UF, Novared 120UFA, Novared 120VFA, Novared 140, Novared 280, Novared C 120, Novared F 5, Novaexcel 140, Novaexcel 150, Novaexcel F 5, Novaexcel ST 100, Novaexcel ST 140, Novaexcel ST 300.

Chemical Considerations: This alternative is an inorganic compound. Red phosphorus refers specifically to the crystalline and amorphous forms of elemental phosphorus which are red in color and consist of random networks of P_4-tetrahedron links. This assessment on red phosphorous does not address other allotropes of elemental phosphorus. White, yellow or black phosphorus do not necessarily have the same properties, fate, or toxicity as red phosphorus. Not all literature entries identify which allotropic form is discussed. (Daubert and Danner, 1989; Kelly, 2006)

Polymeric: The elemental form of red phosphorous produced commercially is an amorphous solid (Brummer, 2005).
Oligomers: Not applicable

Metabolites, Degradates and Transformation Products: Phosphine (CASRN 7803-51-2), phosphorus oxides, hypophosphorus acid (CASRN 6303-21-5), phosphoric acid (CASRN 7664-38-2)

Analog: No analog
Endpoint(s) using analog values: Not applicable

Analog Structure: Not applicable

Structural Alerts: None

Risk Phrases: 11- Highly flammable; 16- Explosive when mixed with oxidizing substances; 52/53- Harmful to aquatic organisms; may cause long-term adverse effects in the aquatic environment (ESIS, 2011). The risk phrases 52/53 is likely to be appropriate only for the yellow/white allotrope of phosphorus which shares a CASRN and an EINECS number with red phosphorus and is generally considered more toxic and reactive than red phosphorus.

Hazard and Risk Assessments: Risk assessment completed for red phosphorus by the Danish Environmental Protection Agency in 2007 (Stuer-Lauridsen et al., 2007) and the Maine Department of Environmental Protection (Maine DEP, 2007).

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.

Red Phosphorus CASRN 7723-14-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	Sublimation point: 416°C (Measured) Triple point: 589.5°C at 43.1 atm	O'Neil, 2010	This substance sublimes.
	Sublimation point: 431°C (Measured) Triple point: 590°C	Lide, 2008	
	>590°C (Measured)	IUCLID, 2000	Inadequate; nonspecific value.
Boiling Point (°C)	Sublimation point: 431°C (Measured) Triple point: 590°C	Lide, 2008	This substance sublimes.
	>400°C (Measured)	IUCLID, 2000	Inadequate; appears to be a cutoff value, and is inconsistent with the reported ability for red phosphorous to sublime.
Vapor Pressure (mm Hg)	0.03 at 21°C (Measured)	Sigma-Aldrich MSDS, 2011	Adequate, consistent values, which span a relatively narrow range.
	0.05 at 25°C (Measured)	EPA, 2010	
	1 at 237°C (Measured)	Spanggord et al., 1983	This value was measured at an elevated temperature.
	<0.075 at 20°C (Measured)	IUCLID, 2000	Inadequate; nonspecific value.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	Professional judgment; EPA, 1999	Based on this chemical's high MW amorphous structure; cutoff value for substances that are not anticipated to display appreciable water solubility according to the HPV assessment guidance.
	Not soluble or insoluble (Measured)	IUCLID, 2000; Stuer-Lauridsen et al., 2007; Lide, 2008	Qualitative descriptions consistent with the low water solubility anticipated for red phosphorous.
	Red phosphorus does not dissolve in water without decomposition (Measured)	Beard, 2000	

Red Phosphorus CASRN 7723-14-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Log K_{ow}			No data located; elemental inorganic materials are outside the estimation domain of EPI estimation models.
Flammability (Flash Point)	Red phosphorus ignites in air at approximately 300°C (Measured)	Diskowski and Hofmann, 2000	Adequate.
	Highly flammable (Measured)	Stuer-Lauridsen et al., 2007	Supporting qualitative value.
	Ignited by friction, static electricity, heating or by oxidizing agents (Measured)	EPA, 2010	Reported in a secondary source, no study details provided.
Explosivity	May explode when exposed to heat or by chemical reaction with oxidizers. It does not react until >260°C. (Measured)	Stuer-Lauridsen et al., 2007	Adequate.
Pyrolysis	Releases phosphorus oxides and phosphorus acids depending on the available oxygen content while burning. (Measured)	Leisewitz et al., 2001	Adequate.
pH	5-6 at 100 g/L and 20˚C (Measured)	IUCLID, 2000	Red phosphorous slowly hydrolyzes to phosphoric acid in the presence of oxygen; therefore the pH of a water solution would be dependent on both its age and concentration.
pK_a		Professional judgment	The substance does not contain functional groups that would be expected to ionize.

Red Phosphorus CASRN 7723-14-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Red phosphorus is not absorbed through the skin and is expected to have poor absorption from the lung and the gastrointestinal tract.**		
Dermal Absorption *in vitro*		Red phosphorus is practically unabsorbable	HSDB, 2011	Reported in a secondary source; limited study details provided.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	Not absorbed from the skin, poor absorption from the lung and gastrointestinal tract (Estimated by analogy)	Professional judgment	Based on analogy to similar compounds.
		Not absorbed through the gastrointestinal tract and, therefore, relatively harmless when ingested	HSDB, 2011	Reported in a secondary source; limited study details provided.
Acute Mammalian Toxicity		**VERY HIGH: Based on oral LD_{50} values of 5 and 11.5 mg/kg in cats and dogs, and, rats and mice, respectively. In addition, mild histological changes in the respiratory tract, respiratory distress, laryngeal lesions and pulmonary congestion have occurred in several animal studies (including human) following exposure to red phosphorus/butyl rubber (RP-BR) smoke at concentrations between 0.1-5.3 mg/L.**		
Acute Lethality	**Oral**	Rat, mouse LD_{50}: 11.5 mg/kg	RTECS; Maine DEP, 2007	Reported in secondary sources.
		Rabbit LD_{50}: 105 mg/kg	RTECS	Reported in a secondary source.
		Cat, dog LD_{50}: 5 mg/kg	RTECS	Reported in a secondary source.
		Rat LD_{50} > 10,000 mg/kg-bw - 15,000 mg/kg-bw	NRC, 1997; Maine DEP, 2007	Reported in secondary sources.
		Single dosage of 0.66 mg/kg did not produce mortality in rabbits or guinea pigs. Cirrhosis-like symptoms were observed.	ERMA; Maine DEP, 2007	Reported in secondary sources.
	Inhalation	Rat, rabbit LC_{Lo} = 0.15 mg/L (150 mg/m^3) Cardiac: EKG changes not diagnostic of specified effects; liver: fatty liver, degeneration; kidney/ureter/bladder - other changes	RTECS	Reported in a secondary source.

Red Phosphorus CASRN 7723-14-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Rat LC_{50} (1 -hour exposures): 2.32-4.3 mg/L (2,320 – 4,300 mg/m^3)	NRC, 1997; Maine DEP, 2007	Reported in secondary sources.
		Sprague Dawley rats and Beagle dogs exposed to RP-BR and black powder mixture at 1.128-1.882 mg/L (1,128-1,882 mg/m^3). Exposure: 60-240 minutes (rats) or 30-240 minutes (dogs) Respiratory distress (leading to prostration and death in some cases). Transient hypoactivity, salivation, conjunctivitis	EPA, 2010	Adequate; however, study details are not available; reported in a secondary source.
		Sprague Dawley rats exposed to an aerosol generated by combustion of RP/BR for 1 or 4 hours. 1 hour exposures: 3.15, 4.33, 5.36 or 8.46 mg/L (3,150, 4,330, 5,360, 8,460 mg/m^3) 4 hour exposure: 1.53 mg/L (1,530 mg/m^3) 1-hour LC_{50} = 4.597 ml/L (4,597 mg/m^3) Slightly-moderately deformed epiglottis (blunted tip or partially to virtually absent, ulceration, edema); laryngeal lesions (severe ulceration and edema with fibrin substance on the mucosal surface of the ventral larynx); moderate-severe pulmonary congestion, edema, hemorrhage.	EPA, 2010	Reported in a secondary source.

Red Phosphorus CASRN 7723-14-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Porton Wistar rats exposed to combustion aerosols of red phosphorus at 3.1 or 3.2 mg/L (3,100 or 3,200 mg/m^3) for 30 minutes. Laryngeal inflammation, blood in tracheal lumen, severe pulmonary congestion and edema, hepatic congestion.	EPA, 2010	Reported in a secondary source.
		Rats, mice, and rabbits exposed to unformulated pure red phosphorus for 1 hour Rat 1-hour LC_{50} = 1.217 mg/L (1,217 mg/m^3) Mouse 1-hour LC_{50} = 0.856 mg/L (856 mg/m^3) Rabbit 1-hour LC_{50} = 5.337 mg/L (5,337 mg/m^3) Death, necrosis and inflammation in the larynx and trachea, pulmonary congestion, hemorrhage, edema, pneumonitis, congestion in liver and kidney (rats, mice guinea pig), cortical necrosis in kidney (mice)	EPA, 2010	Reported in a secondary source.
		Guinea pigs exposed to RP-BR smoke at 120-2.277 mg/L (2,277 mg/m^3) for 5-150 minutes. Death, respiratory distress	EPA, 2010	Reported in a secondary source.

Red Phosphorus CASRN 7723-14-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Mild histological changes in the respiratory tract of rabbits and rats (abnormalities in the larynx and trachea, alveolitis, frank pneumonia) exposed to pyrotechnic mixtures containing red phosphorus	Marrs, 1984	Adequate. Histological effects seem to be a result of orthophosphoric acid aerosol.
		Reversible symptoms of respiratory distress in workers exposed to 0.1-0.7 mg/L (100-700 mg/m^3) red phosphorus smoke for <15 minutes	EPA, 2010	Reported in a secondary source.
Carcinogenicity		**LOW: Estimated not to have potential for carcinogenicity based on expert judgment. Red phosphorus is not listed as a known carcinogen by IARC, NTP, U.S. EPA or CA Prop 65; however, there no long-term carcinogenicity studies were located for red phosphorus smoke.**		
	OncoLogic Results	Low potential for carcinogenicity. (Estimated)	Expert judgment	Estimated based on expert judgment.
	Carcinogenicity (Rat and Mouse)			
	Combined Chronic Toxicity/ Carcinogenicity			
Genotoxicity		**MODERATE: Uncertain potential for mutagenicity based on expert judgment. There is a lack of gene mutation data, genotoxic effects cannot be ruled out. Negative results for both chromosomal aberrations and gene mutation assays are required for a categorization of low.**		
	Gene Mutation *in vitro*	Uncertain potential for mutagenicity. (Estimated)	Expert judgment	Estimated based on expert judgment.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*			No data located.
	Chromosomal Aberrations *in vivo*	Micronucleus test in rat bone marrow polychromatic and normachromatic red blood cells. Weak clastogenic effect in both bone marrow and red blood cells following exposure to 1,000 mg/m^3 for 2 weeks.	NRC, 1997; Maine DEP, 2007	Reported in secondary sources.

Red Phosphorus CASRN 7723-14-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: Estimated not to have potential for reproductive effects based on expert judgment. No adequate data located.**		
	Reproduction/ Developmental Toxicity Screen	Low potential for reproductive effects. (Estimated)	Expert judgment	Estimated based on expert judgment.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Reproduction and Fertility Effects	Sprague Dawley rats exposed to RP-BR smoke at 132 or 1,186 mg/m^3 5 days/week for 10 weeks. No dominant lethal or single generation reproductive effects. No effects on testicular toxicity; however, the fixative used to judge histopathology was not clear. NOAEL = not established.	NRC, 1997	Reported in a secondary source; limited details provided on specific reproductive/fertility parameters measured in the study.

Red Phosphorus CASRN 7723-14-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**LOW: Estimated not to have potential for developmental effects based on expert judgment. No adequate experimental data were located.**		
	Reproduction/ Developmental Toxicity Screen	Low potential for developmental effects. (Estimated)	Expert judgment	Estimated based on expert judgment.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	Pregnant Sprague Dawley rats exposed to RP-BR smoke at 0.132 or 1.183 mg/L (132 or 1,186 mg/m^3) 5 days/week on GD 6-15. No dose-related increases in malformations or variations. Decrease in birth weight.	NRC, 1997	Reported in a secondary source; reproductive endpoints were not fully evaluated; no information on body weight gain, fertility in adults or viability, survival or lactation indices.
	Prenatal Development			No data located.
	Postnatal Development			No data located.
Neurotoxicity		**LOW: Estimated not to have potential for neurotoxicity based on expert judgment. Exposure to red phosphorus/butyl rubber (RB-BR) aerosols increased locomotor activity in rats with incomplete recovery post-exposure.**		
	Neurotoxicity Screening Battery (Adult)	Low potential for neurotoxicity. (Estimated)	Expert judgment	Estimated based on expert judgment.
		Sprague Dawley rats exposed to RP-BR aerosols at 400–1,200 mg/m^3 2.25 hour/day, 4 days/week for 4 weeks; increased motor activity with incomplete recovery after 2 weeks (M). LOAEL = 0.4 mg/L	NRC, 1997	Reported in a secondary source; limited details provided.
	Developmental Neurotoxicity	Phosphorus is classified as a potential developmental neurotoxicant on the Clean Production Action Red List.	Grandjean and Landrigan, 2006	It is unclear if the data pertain to red phosphorus or white phosphorus, which is more toxic.

Red Phosphorus CASRN 7723-14-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects	**LOW: Estimated not to have potential for repeated dose effects based on professional judgment. Experimental toxicity values located are based on inhalation exposure to a pyrotechnic mixture of red phosphorus- and red phosphorus/butyl rubber (RP-BR) smoke and not solely red phosphorous. A LOAEL of 0.015 mg/L for the incidence of aggregates of macrophages containing granules in lungs of mice, severe congestion in the lungs of Guinea pigs, renal disease in mice, rats, and guinea pigs has been identified.**		
	Low potential for repeated dose effects. (Estimated)	Professional judgment	Estimated based on professional judgment.

Red Phosphorus CASRN 7723-14-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Female Portan-strain mice, female Wistar rats and female Dunkin-Hartley guinea pigs exposed to a pyrotechnic mixture of red phosphorus smoke 1 hour/day, 5 days/week for 180 or 200 exposures. Concentrations: 15 and 130 mg/m^3 (0.015–0.13 mg/L) Over 50% of mice died in each dose group; 80% of rats died in the high dose group; 38% of guinea pigs died in the low dose group and all died during or immediately after exposure to the high dose (death appeared due to pulmonary congestion). Depressed growth at both doses (mice, rats). Increased incidence of aggregates of macrophages containing granules in the lungs (mice); severe congestion in the lungs (guinea pigs), though no dose-related changes in rat lungs. Other findings: renal disease (mice, rats, guinea pigs), chronic interstitial nephritis (mice, guinea pigs), nephropathy (rats). LOAEL = 0.015 mg/L	Marrs et al., 1989	Adequate, guideline study.

Red Phosphorus CASRN 7723-14-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Rats (60/group) were exposed to RP-BR smoke at 0, 22, and 165 mg/m^3 (0.022, 0.165 mg/L) for 12 weeks (8 minutes/day, 5 days/week). Reddening and swelling of the eyelids that subsided at study termination.	NRC, 1997	Reported in a secondary source; limited study details provided.

Red Phosphorus CASRN 7723-14-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Rats (Sprague Dawley and Fisher 344) mice (Swiss and A-strain), guinea pigs and rabbits were exposed to 8-43 mg/m^3 (low exposure) or 80-288 mg/m^3 (high exposure) RP-BR 5 days/week for 12 weeks. Daily average exposures were 22 and 165 mg/m^3 (0.022 and 0.165 mg/L) for low and high concentrations, respectively. Increased breathing rate (rats); histological changes in the lungs, trachea, upper respiratory tract and other organs (rats, mice). Authors concluded that these changes were not related to the exposure (sporadic, not unlike what was observed in controls). Morphological lesions in the lung, trachea, nasal turbines, liver, kidney, heart, testes, ovaries, urinary bladder and other organs, however these changes were also seen in controls (guinea pigs, rabbits). NOAEL: 0.165 mg/L (165 mg/m^3) LOAEL: not established as highest concentration tested did not produce adverse effects.	NRC, 1997	Reported in a secondary source.

Red Phosphorus CASRN 7723-14-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Sprague-Dawley rats were exposed to RP-BR aerosols at 400-1,200 mg/m^3 for 2.25 hour/day, 4 days/week for 4 weeks. Wheezing, labored breathing (males at high dose); deceased body weight and food consumption that returned to normal during 14-day recovery period; Pulmonary edema (resolved during recovery); terminal bronchial fibrosis (400 mg/m^3) that did not exhibit recovery during the observation period. LOAEL = 0.4 mg/L (based on terminal incidences of bronchial fibrosis)	NRC, 1997	Reported in a secondary source; limited study details provided.
	Sprague-Dawley (males only) exposed to RP-BR smoke at 50, 180, 300, 750 and 1,200 mg/m^3 for 13 weeks. Most of the animals died during the first 2 weeks of exposure. Decrease in body weight (750 and 1,200 mg/m^3); 10.8% spontaneous death or in moribund state (1,200 mg/m^3); congestion/hemorrhage in lungs; terminal bronchiolar fibrosis and erosions of the laryngeal mucosa with deposition of fibrin on the surface. No deaths at 300 mg/m^3 or less. NOAEL: 0.05 mg/L (50 mg/m^3) LOAEL: 0.18 mg/L (180 mg/m^3) based on incidence of terminal bronchiolar fibrosis	NRC, 1997	Reported in a secondary source.

Red Phosphorus CASRN 7723-14-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Sprague Dawley rats exposed to RP-BR aerosols at 400-1,200 mg/m^3 2.25 hours/day, 4 days/week for 4 weeks. Decreased cholesterol and blood urea (BUN) at (400 mg/m^3, female; 750 mg/m^3, male). Increased triglycerides (400 mg/m^3, female). Female rats exposed to 1,000 mg/m^3 (1 mg/L) had significant decreases in cholesterol and triglycerides and those exposed to 750 mg/m^3 (0.75 mg/L) had decreased BUN after the recovery period. LOAEL = 0.4 mg/L (based on decreased cholesterol and blood urea in female rats)	NRC, 1997	Reported in a secondary source; limited study details provided.
Skin Sensitization		**LOW: Based on experimental data showing a lack of sensitization in guinea pigs.**		
	Skin Sensitization	Not sensitizing, guinea pigs	Maine DEP, 2007	Reported in a secondary source, data are for red phosphorus; limited study details provided.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**MODERATE: Exposure to red phosphorus may cause corneal injury.**		
	Eye Irritation	May cause corneal injury, rabbit (development of numerous fine blood vessels, dilation)	HSDB, 2011	Reported in a secondary source.
		Conjunctivitis, rats (1,813 mg/m^3 for 180 minutes or 1,128 mg/m^3 for 60 minutes) and dogs (1,882 mg/m^3 for 240 minutes) Exposure to red phosphorus smoke. Symptoms resolved within 3 days post-exposure.	NRC, 1997; EPA, 2010	Reported in secondary sources.

Red Phosphorus CASRN 7723-14-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Negative, rabbit (100 mg)	NRC, 1997	Reported in a secondary source.
		Reversible irritation of the eyes and mucous membranes in workers exposed to 0.1-0.7 mg/L (100-700 mg/m^3) red phosphorus smoke for <15 minutes	EPA, 2010	Reported in a secondary source.
Dermal Irritation		**HIGH: Prolonged contact with red phosphorus may cause severe skin irritation.**		
	Dermal Irritation	Negative, guinea pigs (0.5 g on application site)	NRC, 1997	Reported in a secondary source.
		Severe irritation, rabbits Application of RP-BR residue	NRC, 1997	Reported in a secondary source.
		Prolonged or repeated contact may cause skin irritation	Maine DEP, 2007	Reported in a secondary source.
Endocrine Activity		**Estimated not to have potential for endocrine activity based on expert judgment.**		
		Low potential for endocrine activity (Estimated)	Expert judgment	Estimated based on expert judgment.

Red Phosphorus CASRN 7723-14-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Immunotoxicity		**Estimated not to have potential for immunotoxicity based on expert judgment. Exposure to red phosphorus/butyl rubber (RP-BR) aerosols may cause decreases in white blood cell and lymphocyte counts, decreased activity of 5'nucleotides in macrophages, and increased ATP activity.**		
	Immune System Effects	Low potential for immunotoxicity (Estimated)	Expert judgment	Estimated based on expert judgment.
		Sprague Dawley rats exposed to RP-BR aerosols at 400–1,200 mg/m^3 2.25 hours/day, 4 days/week for 4 weeks. Decreased white blood cell count in males and increased blood lymphocytes in females at 750 mg/m^3. Decreased activity of plasma membrane-associated extoenzyme 5'-nucleotidase in macrophages at 750 mg/m^3. Decreased alkaline phosphatase in macrophages after 14-day recovery period (male).	NRC, 1997	Reported in a secondary source; limited study details provided.
		Sprague Dawley rats exposed to RP-BR aerosols 2.25 hour/day, 4 days/week for 13 weeks. Increased ATP levels at 300 mg/m^3; decreased activity of 5'-nucleotidase at 750 mg/m^3,	NRC, 1997	Reported in a secondary source; limited study details provided.
ECOTOXICITY				
ECOSAR Class		Not applicable		

Red Phosphorus CASRN 7723-14-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Acute Toxicity	**LOW: Experimental LC_{50} values are higher than the water solubility of the test substance; no effects at saturation (NES) can be assigned.**		
Fish LC_{50}	96-hour LC_{50} = 33 mg/L	ERMA	Reported in a secondary source; limited study details provided. Effect level higher than the water solubility therefore NES can be predicted.
Daphnid LC_{50}	LC_{50} = 10.5 mg/L	ERMA	Reported in a secondary source; limited study details provided. Effect level higher than the water solubility therefore NES can be predicted.
	48-hour LC_{50} = 1,051 mg/L	Maine DEP, 2007	Reported in a secondary source; limited study details provided. Effect level higher than the water solubility therefore NES can be predicted.
Green Algae EC_{50}	ECb_{50} = 9.5 mg/L	ERMA	Reported in a secondary source; limited study details provided. It is not clear which allotrope of phosphorous was used in this study. Effect level higher than the water solubility therefore NES can be predicted.
Chronic Aquatic Toxicity	**LOW: Experimental toxicity value is higher than the water solubility of the test substance; no effects at saturation NES can be assigned.**		
Fish ChV	*Pimephales promelas* 30-day NOEC) = 0.007 mg/L (0.7 µg/L)	ERMA	Reported in a secondary source; limited study details provided. Effect level higher than the water solubility therefore NES can be predicted.
ENVIRONMENTAL FATE			
Transport	**The low water solubility, relatively low vapor pressure and estimated K_{oc} of >30,000 indicate that red phosphorus will be relatively immobile in the environment and will partition primarily to soil and sediment.**		
Henry's Law Constant ($atm\text{-}m^3$/mole)			This inorganic compound is not amenable to available estimation methods.

Red Phosphorus CASRN 7723-14-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; EPA, 2011b	Cutoff value for non mobile compounds according to SF assessment guidance. This inorganic compound is not amenable to available estimation methods.
	Level III Fugacity Model			Not all input parameters for this model were available for it to be run for this inorganic compound.
Persistence		**HIGH: Red phosphorus is estimated to display high persistence in the environment. Elemental red phosphorus is relatively non reactive under typical environmental conditions. Measured data indicate that red phosphorus will slowly undergo hydrolysis under environmental conditions (<3% in 4 months) and will eventually convert to phosphine and hypophosphorous acid. Subsequent oxidation of these hydrolysis products will lead to the formation of phosphoric oxides and acids.**		
Water	**Aerobic Biodegradation**			No data located; elemental inorganic materials are outside the domain of the EPI estimation models.
	Volatilization Half-life for Model River			No data located.
	Volatilization Half-life for Model Lake			No data located.
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation			No data located.
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.

Red Phosphorus CASRN 7723-14-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Professional judgment	The substance does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
	Hydrolysis	0.7% after 24 hours, 3.7% after 700 hours (Measured)	Walz and Beard, 2000	These non-guideline studies indicate that hydrolysis will occur slowly under environmental conditions.
		Red phosphorus conversion rate of 2.7 % over 4 months at room temperature (Measured)	Walz and Beard, 2000; Stuer-Lauridsen et al., 2007	
		Red phosphorus does not dissolve readily in water; atoms on the surface of the amorphous solid react slowly with water initially forming phosphine (7803-51-2) and hypophosphorous acid (6303-21-5). (Measured)	Leisewitz et al., 2001	
Environmental Half-life				No data located.
Bioaccumulation		**LOW: Due to the large size, water insolubility and amorphous nature of this inorganic substance, elemental phosphorous has a low potential for bioconcentration or bioaccumulation as it is unlikely to pass through biological membranes.**		
	Fish BCF	<100 (Estimated)	Professional judgment	Red phosphorus has very low water solubility. It is also a large, amorphous solid and is unlikely to pass through biological membranes.
	BAF			No data located.
	Metabolism in Fish			No data located.

Red Phosphorus CASRN 7723-14-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL MONITORING AND BIOMONITORING			
Environmental Monitoring	No data located.		
Ecological Biomonitoring	No data located.		
Human Biomonitoring	This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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Resorcinol Bis-Diphenylphosphate

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

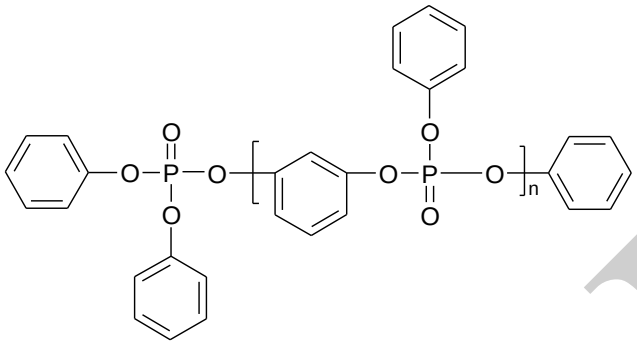
VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from estimation software and professional judgment.

‡ The highest hazard designation of any of the oligomers with MW <1,000.

§ Based on analogy to experimental data for a structural similar compound.

Chemical	CASRN	Human Health Effects										Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Resorcinol Bis-Diphenylphosphate	125997-21-9	L	*M*§	L	L	VL	*M*§	M	*L*		L	VL	VH	*H*‡	M	*H*‡

Resorcinol Bis-Diphenylphosphate



n = 1-7

CASRN: 125997-21-9

MW:
574.46 (n=1);
822.64 (n=2)

MF:
$C_{30}H_{24}O_8P_2$ (n=1);
$C_{42}H_{33}O_{12}P_3$ (n=2)

Physical Forms:
Neat: Liquid

Use: Flame retardant

SMILES: c1ccccc1OP(Oc2ccccc2)(=O)Oc3cccc(c3)OP(=O)(Oc4ccccc4)Oc5ccccc5 (CASRN 57583-54-7; n=1);
c1(OP(=O)(Oc2ccccc2)Oc2ccccc2)cc(OP(=O)(Oc2cc(OP(=O)(Oc3ccccc3)Oc3ccccc3)ccc2)Oc2ccccc2)ccc1 (CASRN 98165-92-5; n=2)

Synonyms: Phosphoric trichloride, polymer with 1,3-benzenediol, phenyl ester (TSCA Inventory); Fyrolflex RDP; Plamtar-RDP; RBBPP; Reofos RDP; Resorcinol bis (biphenyl phosphate); Phosphoric acid, 1,3-phenylene tetraphenyl ester; Phosphorous oxychloride, reaction product with resorcinol and phenol; Resorcinol bis-diphenylphosphate; Tetraphenyl resorcinol diphosphate

Chemical Considerations: This alternative is a polymer; the n=1 and n=2 oligomers are those with a MW <1,000. EPI v4.0 was used to estimate physical/chemical and environmental fate values due to an absence of experimental data. The higher MW oligomers are anticipated to behave similar to the oligomer where n=2.

The material used by industry for flame retardant applications is most likely the polymeric material with CAS number 125997-21-9, although the CAS number for the discrete organic where n=1, 57583-54-7 (Phosphoric acid, P,P'-1,3-phenylene P,P,P',P'-tetraphenyl ester (TSCA Inventory) has been used interchangeably with 125997-21-9 in the publicly available literature.

<table>
<tr><td colspan="2">Polymeric: Yes
Oligomers: The major component of this polymer is the oligomer where n=1, which typically comprises 95-99% of the mixture (U.S. EPA, 2010). The balance is made up of higher oligomers (n=2, 3, etc.) and a triphenyl phosphate impurity (1-5% w/w).</td></tr>
<tr><td colspan="2">Metabolites, Degradates and Transformation Products: Phenol, resorcinol and diphenyl phosphate</td></tr>
<tr><td>Analog: Aryl phosphates and other confidential analogs
Endpoint(s) using analog values: Reproductive Effects; Carcinogenicity; Neurotoxicity; and Repeated Dose Effects</td><td>Analog Structure: The analogs are structural classes or confidential and cannot be suitably represented here.</td></tr>
<tr><td colspan="2">Structural Alerts: Organophosphates, neurotoxicity (U.S. EPA, 2011a).</td></tr>
<tr><td colspan="2">Risk Phrases: Not classified by Annex I Directive 67/548/EEC & IUCLID (Pakalin et al., 2007).</td></tr>
<tr><td colspan="2">Hazard and Risk Assessments: Risk assessment completed for resorcinol bis-diphenylphosphate by Washington State in 2006 (Laflamme, 2006).</td></tr>
<tr><td colspan="2">U.S. EPA TSCA Regulatory Status: 125997-21-9 is listed on the non-confidential TSCA Inventory and is a commenced Premanufacture Notice substance. This chemical is exempt from reporting under the Chemical Data Reporting rule (CDR). 57583-54-7 is not listed on the non-confidential TSCA Inventory.</td></tr>
</table>

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	-12 (Measured)	Akzo Nobel, 1998; Bayer, 2002; Weil, 2001; Supresta, 2011	The reported values are for the pour point of the commercial polymeric mixture, which is a liquid at room temperatures.
	-13 (Measured)	Great Lakes, 2003	
	-16.7 (Measured)	Akzo Nobel, 1998	
Boiling Point (°C)	300 (Measured)	UBA, 2001a, 2003	Decomposition may occur before the boiling point is reached.
	>300 (Measured)	Akzo Nobel, 1998; Bayer, 2002; UBA, 2001b; Supresta, 2011	
	>300 decomposes (Measured)	UBA, 2001b; Great Lakes, 2003	
	370 decomposes (Measured)	Supresta, 2011	
	>400 decomposes (Measured)	Bayer, 2002	
	38 at 138 Pa (Measured)	UBA, 2001a; 2001b, 2003	
Vapor Pressure (mm Hg)	$1.9x10^{-5}$ at 20°C (Measured)	EPA, 2010	The reported experimental data is for the commercial polymeric mixture.
	0.007 at 38°C (Measured)	UBA, 2001a, 2001b, 2003	
	0.28 (Measured)	Supresta, 2011	
	<0.075 at 38°C (Measured)	IUCLID, 2001	
Water Solubility (mg/L)	1.05 mg/L at 20°C (measured)	EPA, 2010	The reported experimental data is for the commercial polymeric mixture.
Log K_{ow}	4.93 (Measured)	EPA, 2010; Wildlife International Ltd., 2003	The reported experimental data is for the commercial polymeric mixture.
	4.9 (Measured)	ICL Industrial, 2009	
Flammability (Flash Point)	>230°C (Measured)	ICL Industrial, 2009	Adequate.
	>240°C (Measured)	Chang Chun	
	302°C (Measured)	Bayer, 2002	
Explosivity	Not explosive (Measured)	IUCLID, 2001; ICL Industrial, 2009	Insufficient study details to assess the quality of this value.
Pyrolysis			No data located.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
pH			Professional judgment	This polymer does not contain functional groups that would be expected to ionize.
pK_a			Professional judgment	This polymer does not contain functional groups that would be expected to ionize.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Poor absorption is predicted for low MW fractions for all routes of exposure.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	Poor absorption is expected for low MW fractions for all routes of exposure.	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/ chemical properties.
Acute Mammalian Toxicity		**LOW: Based on an oral LD_{50} >5,000 mg/kg-bw and a dermal LD_{50} >2,000 mg/kg-bw in rats. The acute inhalation study in rats produced no deaths at the highest dose tested. The LC_{50} of >4.14 mg/L could not be used to evaluate the hazard designation because it is uncertain at which dose the LC_{50} would occur; the criteria threshold for LOW is 5 mg/L for mists. Though unlikely, it is uncertain if the LC_{50} could occur between 4.15 mg/L and 5.0 mg/L (a MODERATE hazard designation).**		
Acute Lethality	**Oral**	Rat Oral LD_{50} >5,000 mg/kg-bw	EPA, 2010	Guideline study reported in a secondary source. Data are for the commercial polymeric mixture.
	Dermal	Rat Dermal LD_{50} >2,000 mg/kg-bw	EPA, 2010	Guideline study reported in a secondary source. Data are for the commercial polymeric mixture.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Inhalation	Rat Inhalation (aerosol, nose-only) LC_{50} >4.14 mg/L	EPA, 2010	The study is a quality guideline study reported in a secondary source; It cannot be used to determine a hazard designation because there were no effects at the highest concentrations tested (4.14 mg/L); From this data, it cannot be determined if effects happened at 4.15 mg/L (MODERATE) or at a concentration that can be considered LOW; therefore, this study cannot be used to determine a hazard designation.
Carcinogenicity		**MODERATE: Estimated to have uncertain potential for carcinogenicity based on analogy to aryl phosphate analogs and professional judgment.**		
	OncoLogic Results			Structure could not be evaluated by OncoLogic.
	Carcinogenicity (Rat and Mouse)	Uncertain potential for oncogenicity (Estimated by analogy)	Professional judgment	Estimated by analogy to aryl phosphates.
	Combined Chronic Toxicity/ Carcinogenicity			No data located.
Genotoxicity		**LOW: Resorcinol bis-diphenylphosphate did not cause gene mutations or chromosomal aberrations *in vitro* and did not produce an increase in micronuclei in mice *in vivo*.**		
	Gene Mutation *in vitro*	Negative in *Salmonella typimurium* (strains not indicated) with and without metabolic activation at concentrations up to 5,000 µg/plate. No cytotoxicity was evident.	Pakalin et al., 2007; EPA, 2010	Guideline study. Data are for the commercial polymeric mixture.
		Negative in *Escherichia coli* (strains not indicated) with and without metabolic activation at concentrations up to 5,000 µg/plate. No cytotoxicity was evident.	Pakalin et al., 2007; EPA, 2010	Guideline study. Data are for the commercial polymeric mixture.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	Negative in chromosomal aberration test (cultured human lymphocytes) with and without metabolic activation at concentrations up to 625 µg/mL. Cytotoxicity data not indicated.	Pakalin et al., 2007; EPA, 2010	Guideline study. Data are for the commercial polymeric mixture.
	Chromosomal Aberrations *in vivo*	Negative in mammalian erythrocyte micronucleus test (swiss mice) following a single oral dose of 5,000 mg/kg-bw.	Pakalin et al., 2007; EPA, 2010	Guideline study. Data are for the commercial polymeric mixture.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: Experimental data for resorcinol bis-diphenylphosphate indicate no adverse effects on reproductive performance or fertility parameters at doses up to 1,000 mg/kg-day (highest dose tested) in a two generation dietary study in rats. There may be potential for reproductive toxicity based on analogy to confidential analog.**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Reproduction and Fertility Effects	Two generation dietary reproduction study in rats. Sprague-Dawley rats (30/sex/dose) were fed 0, 50, 500, or 1,000 mg/kg/day resorcinol bis-diphenylphosphate in the diet for 10 weeks. No clinical signs of toxicity. No effects on litter survival. No adverse effects on any reproductive or fertility parameter measured. No treatment-related lesions in any reproductive organ. NOAEL (parental systemic and reproductive toxicity) = ~ 1,000 mg/kg bw/day LOAEL: not established as highest concentration tested did not produce adverse effects.	Pakalin et al., 2007; EPA, 2010	Guideline study. Data are for the commercial polymeric mixture.
		Potential for reproductive toxicity; no pregnancies (1,000 mg/kg/day); reduced litter size and weight (250 mg/kg/day) NOEL = 50 mg/kg-day LOEL = 205 mg/kg/day (Estimated by analogy)	Professional judgment; Confidential study	Estimated by analogy to confidential analog.
Developmental Effects		**VERY LOW: Resorcinol bis-diphenylphosphate had no toxic or teratogenic/developmental effects at doses up to 1,000 mg/kg-day (highest dose tested) in an oral gavage study in rabbits.**		
	Reproduction/ Developmental Toxicity Screen			No data located.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	Developmental oral gavage study in rabbits. Pregnant New Zealand white rabbits (27/group) were dosed with 200 or 1,000 mg/kg resorcinol bis-diphenylphosphate by oral gavage on GD 6-28. No clinical signs of toxicity. No adverse effects on maternal food consumption, body weight gain or organ weights. No adverse effects on fetal body weights, viability, or any developmental endpoint measured. NOAEL (maternal and developmental toxicity) = 1,000 mg/kg LOAEL: not established as highest concentration tested did not produce adverse effects	EPA, 2010	Guideline study reported in a secondary source. Data are for the commercial polymeric mixture.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Two generation dietary reproduction study in rats. Sprague-Dawley rats (30/sex/dose) were fed 0, 50, 500, or 1,000 mg/kg/day resorcinol bis-diphenylphosphate in the diet for 10 weeks. Vaginal opening and preputial separation were delayed at 500 and 1,000 mg/kg, but effect was considered secondary to reduction of body weight in F_1 generation during week 1 (treated animals had decreased body weights compared to controls during week 1, reportedly due to an initial aversion to taste of diet). NOAEL (parental systemic and developmental toxicity) = ~ 1,000 mg/kg bw/day LOAEL: not established as highest concentration tested did not produce adverse effects.	Pakalin et al., 2007; EPA, 2010	Guideline study. Data are for the commercial polymeric mixture.
	Prenatal Development			No data located.
	Postnatal Development			No data located.
Neurotoxicity		**MODERATE: Estimated to have potential for delayed neurotoxicity based on analogy to aryl phosphate analogs and professional judgment.**		
	Neurotoxicity Screening Battery (Adult)	Potential for delayed neurotoxicity (Estimated by analogy)	Professional judgment	Estimated based on analogy to aryl phosphates.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects	**MODERATE: Experimental data for resorcinol bis-diphenylphosphate reported alveolar histiocytosis in rats following a 4-week inhalation exposure to 0.5 mg/L aerosol (NOAEL = 0.1 mg/L). The criteria threshold for a low hazard designation is 0.2 mg/L for mists based on 90-day repeated dose studies; guidance values are tripled for 28-day study evaluations making the MODERATE hazard range from 0.06 – 0.6 mg/L No other exposure-related gross or microscopic pathology was identified in any organ. There is also potential for liver toxicity based on a confidential analog, though no effects occurred at 300 mg/kg/day for that analog (higher than the criteria threshold for a low hazard designation).**		
Repeated dose effects	28-day oral study, rats Potential for liver toxicity. NOEL = 300 mg/kg/day (Estimated based on analogy)	Professional judgment; Confidential study	Estimated based on analogy to confidential analog.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		In a 4-week inhalation study Sprague-Dawley rats (10/sex/group) were exposed (aerosol, nose only) to 0, 100, 500 or 2,000 mg/m^3 (0, 0.1, 0.5, or 2 mg/L) resorcinol bis-diphenylphosphate. No deaths or clinical signs of toxicity. Decreased body weight and food consumption in males and significant inhibition of plasma cholinesterase in females at 2,000 mg/m^3. White foci in the lungs at 2,000 mg/m^3 and alveolar histiocytosis at 500 and 2,000 mg/m^3. Although lung changes are relevant, they were not considered to be a reflection of a specific toxic response to resorcinol bis-diphenylphosphate; these changes are characteristic of exposure to non-cytotoxic water-insoluble materials. No other gross or microscopic pathology in any organ. NOAEC: 100 mg/m^3 (0.1 mg/L) LOAEC: 500 mg/m^3 (0.5 mg/L) based on alveolar histiocytosis	EPA, 2010	Guideline study reported in a secondary source. Data are for the commercial polymeric mixture.
Skin Sensitization		**LOW: Estimated to not have potential for skin sensitization based on expert judgment.**		
	Skin Sensitization	No potential for skin sensitization (Estimated)	Expert judgment	Estimated by expert judgment.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Resorcinol bis-diphenylphosphate produced mild irritation in rabbit eyes; however, clearing occurred within 24 hours.**		

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Eye Irritation	Rabbit, minimally irritating. 0.1 ml instilled into the left eyes of 3 rabbits produced slight conjunctival redness and chemosis that was reversible by 24 hours.	EPA, 2010	Guideline study reported in a secondary source. Data are for the commercial polymeric mixture.
Dermal Irritation		**VERY LOW: Resorcinol bis-diphenylphosphate was not a dermal irritant in rabbits.**		
	Dermal Irritation	Rabbit, not irritating	EPA, 2010	Guideline study reported in a secondary source. Data are for the commercial polymeric mixture.
Endocrine Activity		**No data located.**		
				No data located.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Immunotoxicity		**Resorcinol bis-diphenylphosphate had no effect on immunological parameters at doses up to 5,000 mg/kg-day (highest dose tested) in an oral gavage study in mice.**		
	Immune System Effects	Negative, oral gavage study in mice. Female B6C3F1 mice (50/group) were exposed via oral gavage to 0, 500, 1,500, or 5,000 mg/kg-day resorcinol bis-diphenylphosphate for 28 days. No deaths, clinical signs of toxicity, or effects on body or organ weights. No adverse histopathological changes or necropsy findings. No treatment-related changes in peritoneal cell numbers or cell types, peritoneal macrophage phagocytic activity or host susceptibility to infection. No adverse effect on splenic natural killer cell activity, lymphocyte blastogenesis, or antibody-forming cell function. There were significant decreases in erythrocyte cholinesterase activity and plasma pseudocholinesterase activity in all dose groups, but both enzyme activities returned to control levels at the end of the 60 day recovery period. NOAEL: 5,000 mg/kg-day LOAEL: not established, as highest dose tested did not produced adverse effects.	EPA, 2010	Guideline study reported in a secondary source. Data are for the commercial polymeric mixture.
ECOTOXICITY				
ECOSAR Class		Esters; Esters (phosphate)		
Acute Toxicity		**VERY HIGH: Based on measured EC_{50} values for daphnia. Measured values for fish and algae are higher than the water solubility limit, suggesting no effects at saturation (NES).**		

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Fish LC_{50}	*Brachydanio rerio* 96-hour LC_{50} = 12.3 mg/L	EPA, 2010	Guideline study reported in a secondary source (OECD Guide-line 203). Data are for the commercial polymeric mixture. Given that the reported value is greater than the water solubility, NES were observed for this endpoint.
Daphnid LC_{50}	*Dapnhia magna* 48-hour EC_{50} = 0.7 mg/L	EPA, 2010	Guideline study reported in a secondary source (U.S. EPA OPPTS 850.1010). Data are for the commercial polymeric mixture.
Other Freshwater Invertebrate LC_{50}	Mysid shrimp 96-hour LC_{50} = 0.005 mg/L Mysid shrimp 96-hour LC_{50} = $5.16x10^{-5}$ mg/L ECOSAR: Esters	EPI	Estimates were performed on representative components of the polymer that have a MW <1,000.
	Mysid shrimp 96-hour LC_{50} = $5.16x10^{-5}$ mg/L ECOSAR: Esters	EPI	Estimates were performed on representative components of the polymer that have a MW < 1,000.
Green Algae EC_{50}	*Pseudokirchneriella subcapitata* 72-hour EC_{50} = 48.6 mg/L	EPA, 2010	Guideline study reported in a secondary source (OECD 201). Data are for the commercial polymeric mixture. Given that the reported value is greater than the water solubility, NES was observed for this endpoint.
Chronic Aquatic Toxicity	**HIGH: Based on an estimated ChV value for the n = 1 oligomer (phosphate esters ECOSAR class) of 0.0093 mg/L for fish.**		
Fish ChV	32/33-d ChV = 0.00155 mg/L (n=1) ECOSAR: Esters	EPI	Estimates were performed on representative components of the polymer that have a MW <1,000; data are for the n=1 oligomer.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	32/33-d ChV = $3.27x10^{-5}$ mg/L (n=2) ECOSAR: Esters	EPI	Estimates were performed on representative components of the polymer that have a MW <1,000; data are for the n=2 oligomer; NES are estimated for representative component of the polymer with a MW <1,000.
	ChV = 0.00093 mg/L (n=1) ChV = $8.53x10^{-6}$ mg/L (n=2) ECOSAR: phosphate esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES are estimated for the n=2 and higher oligomers.
	ChV = $8.53x10^{-6}$ mg/L (n=2) ECOSAR: phosphate esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES are estimated for the n=2 and higher oligomers.
Daphnid ChV	21-day ChV = 0.010 mg/L (n=1) ECOSAR: Esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES are estimated for the n=2 and higher oligomers.
	21-day ChV = 0.000145 mg/L (n=2) ECOSAR: Esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES are estimated for the n=2 and higher oligomers.
	ChV = 0.004 mg/L (n=1) ChV = $3.27x10^{-5}$ mg/L (n=2) ECOSAR: phosphate esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES are estimated for the n=2 and higher oligomers.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	ChV = $3.27x10^{-5}$ mg/L (n=2) ECOSAR: phosphate esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES are estimated for the n=2 and higher oligomers.
Saltwater Invertebrate ChV	Mysid shrimp 96-hour LC_{50} = $4.79x10^{-6}$ mg/L (n=1) Mysid shrimp 96-hour LC_{50} = $1.61x10^{-10}$ mg/L (n=2) ECOSAR: Esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES are estimated for the n=2 and higher oligomers.
	Mysid shrimp 96-hour LC_{50} = $1.61x10^{-10}$ mg/L (n=2) ECOSAR: Esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES are estimated for the n=2 and higher oligomers.
Green Algae ChV	ChV = 0.023 mg/L (n=1) ECOSAR: Esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES are estimated for the n=1 and higher oligomers.
	ChV = 0.00116 mg/L (n=2) ECOSAR: Esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES are estimated for the n=2 and higher oligomers.
	ChV = 0.166 mg/L (n=1) ChV = $3.39x10^{-5}$ mg/L (n=2) ECOSAR: phosphate esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES estimated for the n=2 and higher oligomers.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		ChV = $3.39x10^{-5}$ mg/L (n=2) ECOSAR: phosphate esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; NES estimated for the n=2 and higher oligomers.
Earthworm Subchronic Toxicity		14-day LC_{50} = 135.164 mg/L (n=1) 14-day LC_{50} = 25.935 mg/L (n=2) ECOSAR: Esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000; data are for the n=1 oligomer.
		14-day LC_{50} = 25.935 mg/L (n=2) ECOSAR: Esters	EPI	Estimates were performed on oligomers of the polymeric mixture that have a MW <1,000.
ENVIRONMENTAL FATE				
Transport		**The environmental fate is described for the oligomer where n=1, which is the primary component of the commercial product. Based on the Level III fugacity models incorporating the located experimental property data, resorcinol bis-diphenylphosphate is expected to partition primarily to soil and sediment. Resorcinol bis-diphenylphosphate is expected to be immobile in soil based on its estimated K_{oc}. Leaching of resorcinol bis-diphenylphosphate through soil to groundwater is not expected to be an important transport mechanism. Estimated volatilization half-lives indicate that it will be non-volatile from surface water. Volatilization from dry surface is also not expected based on its vapor pressure. In the atmosphere, resorcinol bis-diphenylphosphate is expected to exist solely in the particulate phase, based on its estimated vapor pressure. Particulates may be removed from air by wet or dry deposition. The higher MW components of the commercial product are anticipated to behave similarly to that described above.**		
	Henry's Law Constant (atm-m^3/mole)	<10^{-8} (Estimated for n=1 and n=2)	EPI; EPA, 2011b	Cutoff value for non volatile compounds according to SF assessment guidance. Higher MW components are also expected to have Henry's Law Constant values below this cutoff.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated for n=1 and n=2)	EPI; EPA, 2011b	Cutoff value for non mobile compounds according to SF assessment guidance. Higher MW components are also expected to have K_{oc} values above this cutoff.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Level III Fugacity Model	Air = <1% (Estimated for n=1) Water = 1% Soil = 40% Sediment = 59% Air = <1% (Estimated for n=2) Water = 1% Soil = 42% Sediment = 57%	EPI	Estimates were performed on representative components of the polymer.
Persistence		**MODERATE: Moderate persistence is expected for resorcinol bis-diphenylphosphate based on experimental biodegradation studies that indicate the potential for biodegradation of the commercial polymeric mixture. The commercial mixture was determined to be inherently biodegradable using the guidelines of Directive 84/449/EEC, C.6 "Biotic degradation - the Closed Bottle test" test. After 28 days, 37% biodegradation occurred and after 56 days, 66% biodegradation occurred. Resorcinol bis-diphenylphosphate oligomers (n=1 and n=2) do not contain chromophores that absorb at wavelengths >290 nm, and therefore, are not expected to be susceptible to direct photolysis by sunlight. The atmospheric half-life of resorcinol bis-diphenylphosphate oligomers are estimated to be 6.1 (n=1) and 4.1 (n=2) hours, although they are expected to exist primarily in the particulate phase in air. Additionally, resorcinol bis-diphenylphosphate is estimated to undergo hydrolysis slowly under neutral and acidic conditions.**		
Water	**Aerobic Biodegradation**	37% degradation after 28 days; 66% degradation after 56 days Using Directive 84/449/EEC, C.6 (Measured) inherent biodegradation, 2.7 mg/L of compound in activated sludge	IUCLID, 2001	The data is for the commercial polymeric mixture (CASRN 125997-21-9).
	Volatilization Half-life for Model River	>1 year (Estimated for n=1 and n=2)	EPI	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated for n=1 and n=2)	EPI	Based on the magnitude of the estimated Henry's Law Constant.
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation	Not probable (Anaerobic-methanogenic biodegradation probability model for n=1 and n=2)	EPI	

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	6.1 hours (Estimated for n=1) 4.1 hours (Estimated for n=2)	EPI	
Reactivity	**Photolysis**	Not a significant fate process (Estimated for n=1 and n=2)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
	Hydrolysis	Half-life = 320 days at pH 7 Half-life = 32 days at pH 8 Half-life = 3 days pH 9 (Estimated for n=1) Half-life = 240-320 days at pH 7 Half-life = 24-32 days at pH 8 Half-life = 2-3 days pH 9 (Estimated for n=2)	EPI	
		Half-life = 11 days (20°C; pH 4) Half-life = 17 days (20°C; pH 7) Half-life = 21 days (20°C; pH 9) OECD 111 (Measured)	IUCLID, 2001	Inadequate. Although reported as a guideline study, phosphate esters as a chemical class have been observed to hydrolyze more rapidly under basic pHs then under neutral or acidic conditions. The reported half-lives do not follow this trend, and are therefore suspect.
Environmental Half-life		>180 days (Estimated for n=1 and n=2)	EPI; PBT Profiler	Half-life estimated for the predominant compartment, as determined by EPI and the PBT Profiler methodology.

Resorcinol Bis-Diphenylphosphate CASRN 125997-21-9				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Bioaccumulation		**HIGH: The estimated BCF value for the n=1 component has high potential for bioaccumulation. The higher MW oligomers that may be found in this mixture (n=2, 3, 4…) are expected to have moderate or low potential for bioaccumulation based on their large size and low solubility according to the Sustainable Futures (SF) polymer assessment guidance (U.S. EPA, 2010).**		
	Fish BCF	1,300 (Estimated for n=1) 59 (Estimated for n=2)	EPI	
	BAF	81 (Estimated for n=1) 7 (Estimated for n=2)	EPI	
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the biomonitoring report (CDC, 2011).		

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Substituted Amine Phosphate Mixture

Screening Level Hazard Summary

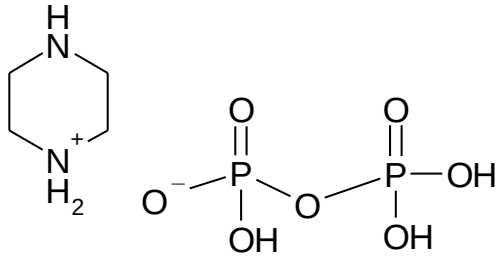
This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.
§ Based on analogy to experimental data for a structurally similar compound.

		Human Health Effects											Aquatic Toxicity		Environmental Fate	
Chemical	**CASRN**	**Acute Toxicity**	**Carcinogenicity**	**Genotoxicity**	**Reproductive**	**Developmental**	**Neurological**	**Repeated Dose**	**Skin Sensitization**	**Respiratory Sensitization**	**Eye Irritation**	**Dermal Irritation**	**Acute**	**Chronic**	**Persistence**	**Bioaccumulation**
Substituted Amine Phosphate Mixture[1]	Confidential	***H***	***M***	***M***	***M***	***M***	***L***	***M***	***M***	***M*§**	***L*§**	***VH***	***M***	***L***	***H***	***L***

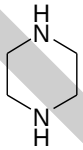
[1] Hazard designations are based upon the component of the salt with the highest hazard designation, including the corresponding free acid or base.

Substituted Amine Phosphate Mixture



mixture with confidential substituted amine phosphate

	CASRN: 66034-17-1 (Piperazine pyrophosphate) and confidential CASRN (substituted amine phosphate)
	MW: 264 (Piperazine pyrophosphate) and confidential MW (substituted amine phosphate)
	MF: $C_4H_{11}N_2^{+1} \cdot P_2O_7H_3^{-1}$ and confidential MF (substituted amine phosphate)
	Physical Forms: **Neat:** Solid
	Use: Flame retardant
SMILES: This mixture containing confidential material is not amenable to the generation of a single SMILES notation.	
Synonyms: ADK STABILIZER FP-2100J; ADK STABILIZER FP-2200; ADK STABILIZER FP-2200S; ADK STABILIZER FP-2400	
Chemical Considerations: This alternative is a mixture. The substituted amine phosphate mixture represents the ADK Stabilizer series of commercial mixtures that are comprised of approximately 50% of piperazine pyrophosphate (Diphosphoric acid, compd. with piperazine (1:1), CAS 66034-17-1, MW=264) and a substituted amine phosphate. Piperazine pyrophosphate will dissociate into piperazine and pyrophosphate (diphosphoric acid) anions under environmental conditions and, therefore, the relevant dissociation products piperazine or pyrophosphate was used in each endpoint as appropriate. The same approach was used for the substituted amine phosphate anions. Measured or estimated values for the dissociated components were used to fill assessment data gaps as appropriate.	

Polymeric: No **Oligomers:** Not applicable	
Metabolites, Degradates and Transformation Products: Pyrophosphoric acid (2466-09-3), Piperazine (110-85-0), glycine (56-40-6) and other confidential substances.	
Analog: Piperazine (110-85-0); and confidential analogs, piperazine-containing compounds. **Endpoint(s) using analog values:** Eye irritation; respiratory sensitization, skin sensitization, eye and skin irritation	**Structure:**  Piperazine
Structural Alerts: Amines, potential nephrotoxins (U.S. EPA, 2011a).	
Risk Phrases: Not classified by Annex VI Regulation (EC) No. 1272/2008 (ESIS, 2011).	
Hazard and Risk Assessments: None	
U.S. EPA TSCA Regulatory Status: For piperazine pyrophosphate: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory and is a commenced Premanufacture Notice substance that contained a Significant New Use Rule regulating the chemical as follows: this product cannot be released into U.S. Waters.	

Substituted Amine Phosphate Mixture			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	>300 (Estimated)	Professional judgment	The components of this mixture are ionic compounds and are anticipated to be high melting solids. Cutoff value for high melting compounds.
Boiling Point (°C)	>270 decomposes (Measured)	Adeka, 2011	Product information for FP-2100J; refers to the ionic compounds in ADK stabilizers.
	>260 decomposes (Measured)	Adeka, 2011	Product information for FP-2200; refers to the ionic compounds in ADK stabilizers.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2011b	Cutoff value for nonvolatile compounds according to SF assessment guidance. Applies to both ionic solids present in the substituted amine phosphate mixture.
Water Solubility (mg/L)	**Piperazine pyrophosphate:** >1,000,000 (Estimated)	EPI	
	Substituted amine phosphate component: >1,000,000 (Estimated)	EPI	
	Substituted amine phosphate component: approximately 800; 900 (Measured)	Confidential MSDS, 2011; Weil, 2001	Inadequate; these reported values are inconsistent with structurally similar phosphates.
Log K_{ow}	**Piperazine pyrophosphate:** <-2 (Estimated)	EPI	
	Substituted amine phosphate component: <-2 (Estimated)	EPI	

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Flammability (Flash Point)		Non flammable (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Explosivity		Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis				No data located.
pH				No data located.
pK_a				No data located.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**No toxicokinetic data were located for the substituted amine phosphate mixture. The substituted amine phosphate mixture is estimated to not be absorbed through the skin and absorption is expected through the lung and gastrointestinal (GI) tract. Following absorption, limited data suggest distribution throughout the GI system, liver, and kidney for the substituted amine phosphate and piperazine components. Data for the substituted amine phosphate component indicate an elimination phase half-life of 2.7 hours from plasma and 3 hours for urine. Data for the piperazine component indicate rapid elimination from blood and kidney.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	**Substituted amine phosphate mixture:** Not absorbed from the skin, absorption through lung and GI tract. (Estimated by analogy)	Professional judgment	Based on closely related analogs with similar structures, functional groups, and physical/chemical properties.
		Substituted amine phosphate component: The elimination phase half-life calculated from plasma data was 2.7 hours, and the urinary half-life was 3.0 hours. The renal clearance was determined to be 2.5 mL/min. (Measured for the free base)	Confidential study	Nonguideline study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Substituted amine phosphate component: Distributed to stomach, small intestine, cecum, and large intestine, and found in blood, and urine of rats. (Measured for the free base)	Confidential study	Study details reported in a secondary source.
		Piperazine: pig, oral (gavage); peak plasma concentrations occurred 1 hour after exposure; quickly eliminated from blood. Distributed primarily to kidneys and liver; eliminated quickly from kidney, and slower from liver, skeleton, muscle, fat and skin. Low potential for bioaccumulation. (Measured for the free base)	ECHA, 2011	Study details reported in a secondary source.
Acute Mammalian Toxicity		**HIGH: Using a conservative approach, acute toxicity hazard potential for the substituted amine phosphate mixture is estimated based on toxicity for inhalation exposure to the piperazine moiety in rats. The hazard is estimated to be low for oral and dermal routes of exposure to the substituted amine phosphate and piperazine components of the mixture.**		
Acute Lethality	**Oral**	**Substituted amine phosphate component:** Rat LD_{50} = 3,161 mg/kg b.w. (male), 3,828 mg/kg (females) (Measured for the free base)	Confidential study	Adequate.
		Substituted amine phosphate component: Mouse LD_{50} = 3,296 mg/kg (male), 7,014 mg/kg (female) (Measured for the free base)	Confidential study	Adequate.
		Substituted amine phosphate component: Mouse LD_{50} = 4,550 mg/kg (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: Rat LD_{50} = 3,160 mg/kg (male) and 3850 mg/kg (female) (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Substituted amine phosphate component: Rat LD_{50} >6,400 mg/kg (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: LD_{50} ≈ 4,800 mg/kg	Confidential study	Limited study details reported in a confidential study.
		Piperazine: Rat LD_{50} = 1,900–4,500 mg/kg (Measured)	IUCLID, 2000	Reported results taken from 3 studies. Limited study details reported in a secondary source.
		Piperazine: Mouse LD_{50} = 600–4,200 mg/kg (Measured)	IUCLID, 2000	Reported results taken from 3 studies. Limited study details reported in a secondary source.
		Piperazine: Rat LD_{50} = 2,500 mg/kg (Measured)	ECHA, 2011	Study details reported in a secondary source; according to OECD Guideline 401.
		Piperazine: Rat LD_{50} = 3,200 mg/kg (Measured)	ECHA, 2011	Study details reported in secondary source; according to OECD Guideline 401.
		Piperazine: Rat LD_{50} = 2,600 mg/kg (Measured)	ECHA, 2011	Study details reported in secondary source; according to OECD Guideline 401.
	Dermal	**Piperazine:** Rabbit LD_{50} = 4,000 mg/L	ECHA, 2011	Limited study details provided in a secondary source.
		Substituted amine phosphate component: Rabbit LD_{50} >1,000 mg/L (Measured)	Confidential study	Limited study details reported in a confidential study.
	Inhalation	**Substituted amine phosphate component:** Rat LC_{50} = 3.248 mg/L (Measured)	Confidential study	Study details, if present, were not translated into English; reported in a confidential study.
		Piperazine: Rat 4-hour LC_{50} = 2.0 mg/L (Measured)	ECHA, 2011	Study details reported in secondary source.
		Piperazine: Rat 4-hour LC_{50} = 0.8 mg/L (Measured)	ECHA, 2011	Study details reported in secondary source.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Piperazine: Rat 2-hour LC_{50} = 5.4 mg/L. (Measured)	IUCLID, 2000	Limited study details reported In a secondary source.
Carcinogenicity		**MODERATE: The carcinogenicity hazard potential for the substituted amine phosphate mixture is estimated to be moderate based on the substituted amine phosphate component. There is evidence that oral exposure to the substituted amine phosphate component causes carcinogenicity in experimental animals. However, there is no evidence located as to the substituted amine phosphate component's carcinogenicity to humans. Tumor formation in animals appeared to happen in a mechanical nature under conditions in which it produced bladder calculi. No data were located as to the carcinogenic potential of the substituted amine phosphate mixture or salts. IARC classifies the substituted amine phosphate component as Group 3*: not classifiable as to its carcinogenicity to humans.***		
	OncoLogic Results	**Substituted amine phosphate component:** Marginal (Estimated for free base)	OncoLogic	
	Carcinogenicity (Rat and Mouse)	**Substituted amine phosphate component:** Group 3: *It is not classifiable as to its carcinogenicity to humans*; there is inadequate evidence in humans for carcinogenicity, and there is sufficient evidence in experimental animals for carcinogenicity under conditions in which it produces bladder calculi. (Measured for the free base)	Confidential study	Classification statement.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Substituted amine phosphate component: Significant formation of transitional cell carcinomas in the urinary bladder of male rats and significant chronic inflammation in the kidney of dosed female rats were observed following exposure in the feed for up to 103 weeks. Carcinoma formation was significantly correlated with the incidence of bladder stones. A transitional-cell papilloma was observed in the urinary bladder of a single high dose male rat, and compound related lesions were observed in the urinary tract of dosed animals. Based on the mechanical nature of tumor formation, FDA and EPA considered it noncarcinogenic. (Measured for the free base)	Confidential study	Reported in a confidential study.
		Substituted amine phosphate component: Increased incidence of acute and chronic inflammation and epithelial hyperplasia of the urinary bladder were observed in male mice following oral (feed) exposure for up to 103 weeks. Bladder stones and compound related lesions were observed in the urinary tract of test animals. There was no evidence of bladder tumor development. The compound was not considered carcinogenic. (Measured for the free base)	Confidential study	Reported in a confidential study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Substituted amine phosphate component: Proliferative lesions of the rat urinary tract were directly due to the irritant stimulation of calculi, and not to molecular interactions between it or its metabolites with the bladder epithelium. (Measured for the free base)	Confidential study	Reported in a confidential study.
		Substituted amine phosphate component: Water intake, used as an index of urinary output, was increased by NaCl treatment. Calculus formation resulting from administration was suppressed dose-dependently by the simultaneous NaCl treatment. The main constituents of calculi were the substituted amine phosphate component and uric acid (total contents 61.1–81.2%). The results indicated proliferative lesions of the urinary tract of rats were directly due to the irritation-induced stimulation of calculi, and not molecular interactions between itself or its metabolites with the bladder epithelium. (Measured for the free base)	Confidential study	Reported in a confidential study.
		Substituted amine phosphate component: As an initiator, it caused no significant increase in papillomas per mouse when compared to controls.	Confidential study	Reported in a confidential study;; nonguideline study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Substituted amine phosphate component: Diffuse papillary hyperplasia of the bladder epithelium and bladder calculi were observed in all the treated rats. Elevated spermidine/spermine N1-acetyltransferase activity following treatment was considered to be an indicator of cell proliferation. (Measured for the free base)	Confidential study	Reported in a confidential study; nonguideline study.
		Substituted amine phosphate component: Decreased antitumor activity was correlated with increasing demethylation; the component was considered inactive as an antitumor drug. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: In an *in vitro* cytotoxicity study in cultured ADJ/PC6 plasmacytoma ascites tumor cells, the ID_{50} was 470 μg/mL after 72 hours of treatment. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
	Combined Chronic Toxicity/ Carcinogenicity	**Substituted amine phosphate component:** No effects were observed in rats fed 1,000 ppm. 4 of the 10 rats fed 10,000 ppm had bladder stones associated with the development of benign papillomata. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Substituted amine phosphate component: Increased incidence of urinary bladder stones (6/20 rats) was noted in the 10,000 ppm dose group, and was associated with an increase in benign papillomata. The NOAEL was determined to be 1,000 ppm (67 mg/kg). (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
Genotoxicity		**MODERATE: Estimated based on positive results for chromosomal aberrations *in vivo* in mice exposed to the substituted amine phosphate component and positive results for gene mutations following *in vitro* exposure to the piperazine component in mouse lymphoma assays. There were also positive results *in vitro* for DNA synthesis-inhibition in Hela S3 cell and genetic toxicity in *Escherichia coli* WP2s in a microscreen assay following exposure to the substituted amine phosphate component. No data were located for the substituted amine phosphate mixture salts regarding the genotoxicity endpoint.**		
	Gene Mutation *in vitro*	**Substituted amine phosphate component:** Bacterial forward mutation assay: Negative with and without liver activation (Measured for the free base)	Confidential study	Reported in a confidential study.
		Substituted amine phosphate component: Bacterial forward mutation assay: Negative (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: Bacterial reverse mutation assay: Negative with and without liver activation (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: Bacterial reverse mutation assay: Negative with and without unspecified metabolic activation (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Substituted amine phosphate component: *In vitro* mouse lymphoma test: Negative with and without liver activation (Measured for the free base)	Confidential study	Reported in a confidential study.
		Substituted amine phosphate component: CHO/HGPRT forward mutation assay: Negative with and without liver activation (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Piperazine: *S. typhimurium* TA98, TA100, TA1535, TA1537 gene mutation assay: Negative with and without metabolic activation (Measured for the free base)	IUCLID, 2000; ECHA, 2011	Study details reported in a secondary source; according to OECD Guideline 471.
		Piperazine: *E. coli* reverse mutation assay: Negative without metabolic activation	IUCLID, 2000	Results taken from several studies. Limited study details reported in a secondary source.
		Piperazine: Mouse lymphoma assay: positive	IUCLID, 2000	Limited study details reported in a secondary source.
		Piperazine: Mammalian cell gene mutation assay; mouse lymphoma L5178Y cells; toxicity-related increases in gene mutations in the presence of metabolic activation and negative without metabolic activation	ECHA, 2011	Study details reported in secondary source; equivalent to OECD Guideline 476; test substance identified as piperazine polyphosphate.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Gene Mutation *in vivo*	**Substituted amine phosphate component:** *In vivo* mouse micronucleus test: The initial test gave a positive trend (P=0.003) for chromosomal damage; however, both peripheral blood smears and the repeat bone marrow test were negative. The overall conclusion was that the substituted amine phosphate component does not induce chromosomal damage. (Measured for the free base)	Confidential study	Reported in a confidential study.
		Substituted amine phosphate component: *In vivo* mouse micronucleus test: Negative without activation (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Piperazine: *E. coli* reverse mutation assay: Negative without metabolic activation (Measured)	IUCLID, 2000	Results taken from several studies. Limited study details reported in a secondary source.
	Chromosomal Aberrations *in vitro*	**Substituted amine phosphate component:** *In vitro* chromosomal aberrations test: Negative in Chinese hamster ovary (CHO) cells with and without liver activation (Measured for the free base)	Confidential study	Reported in a confidential study.
		Substituted amine phosphate component: *In vitro* sister chromatid exchange assay: Negative in CHO cells with and without liver activation (Measured for the free base)	Confidential study	Reported in a confidential study..
		Substituted amine phosphate component: *In vitro* sister chromatid exchange assay: Negative in CHO cells with and without liver activation (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Piperazine: Chromosomal aberration assay: Negative in CHO cells with and without metabolic activation	ECHA, 2011	Study details reported in secondary source; equivalent to OECD Guideline 473.
	Chromosomal Aberrations *in vivo*	**Substituted amine phosphate component:** *In vivo* chromosome aberrations test in mice: Positive (Measured for the free base)	Confidential study	Reported in a confidential study.
	DNA Damage and Repair	**Substituted amine phosphate component:** *In vivo* and *in vitro* unscheduled DNA synthesis (UDS) test: None of the tested chemicals, including the substituted amine phosphate component were genotoxic hepatocarcinogens in the *in vivo* assay, They were also negative for UDS in the *in vitro* assay (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: SOS/*umu* test: Negative for its ability to result in DNA damage and induce the expression of the *umu* operon	Confidential study	Reported in a confidential study; nonguideline study.
		Substituted amine phosphate component: DNA synthesis-inhibition test in Hela S3 cells: Inhibits DNA synthesis by 50% (DI_{50}) at greater than 300 μM (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Other	**Substituted amine phosphate component:** Sex-linked recessive lethal/reciprocal translocation: Results were considered equivocal based on 0.18% and 0.36% total lethality following oral and injection exposure, respectively, compared to control total lethal of 0.07% for oral and 0.09% for injection (Measured for the free base)	Confidential study	Reported in a confidential study.
		Substituted amine phosphate component: *Drosophila* Muller-5 test: Negative for mutagenicity (Measured for the free base)	Confidential study	Insufficient study details were reported in a confidential study.
		Substituted amine phosphate component: *Drosophila melanogaster* Sex-linked recessive lethal: No mutagenic effects were observed (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: *In vitro* flow cytometric DNA repair assay: Negative for genotoxic effects (Measured for the free base)	Confidential study	Reported in a confidential study; nonguideline study.
		Substituted amine phosphate component: Microscreen assay: Positive for genetic toxicity in *E.coli* WP2 cells	Confidential study	Reported in a confidential study; nonguideline study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Substituted amine phosphate component: Growth and genotoxic effects to bacteria (*Salmonella typhimurium)* and yeast *(Saccharomyces cerevisiae)*: Non-mutagenic in *S.typhimurium* with or without S-9 mix. The growth of eight out of nine strains tested was delayed by 10 mM during 24 hr cultivation. *S.cerevisiae* strain was tested, and did not recover its growth following 48 hour cultivation. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Piperazine: Mammalian cell transformation test: Negative in mouse BALB/3T3 cells; piperazine did not induce transformed foci (Measured)	ECHA, 2011	Study details reported in secondary source; according to EU method B.21.
Reproductive Effects		**MODERATE: Hazard potential for reproductive toxicity of the substituted amine phosphate mixture is estimated to be moderate based on data for the piperazine moiety from piperazine dihydrochloride; rats exposed to 300 mg/kg/day had decreased litter size in both generations. The NOAEL is identified at 125 mg/kg/day; there is uncertainly if effects could occur at doses between 125 and 250 mg/kg/day (the criteria cutoff dose for a LOW hazard designation is > 250 mg/kg/day. There were no adequate reproductive toxicity data located for the substituted amine phosphate mixture or substituted amine phosphate component of the mixture were located.**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Reproduction and Fertility Effects	**Piperazine:** Rat, oral, 2-generation reproduction toxicity study; at 300 mg/kg/day: Decreased body weight gain in F0 males and in both sexes of F1 parental generation; no effect on number of pregnancies; decreased litter size in both generations (91% - F0, 85%-F1 offspring); reduction of implantation sites in F1 females; no difference in offspring sex ratios. NOAEL = 227 mg/kg/day piperazine dihydrochloride (~125 mg/kg/day piperazine base) LOAEL = 544 mg/kg/day piperazine dihydrochloride (~300 mg/kg/day piperazine base)	ECHA, 2011	Reported in a secondary source. Test substance identified as piperazine dihydrochloride.
		Piperazine: Rat, oral; concern for reproductive toxicity NOAEL = 250 mg/kg/day	Professional judgment; Confidential study	Test substance is identified as piperazine dihydrochloride; a LOAEL was not identified. Reported in a confidential study.
		Substituted amine phosphate component: There were no treatment-related macroscopic or microscopic effects on mammary glands, ovaries, prostate, seminal vesicles, testes and uterus in rats and mice in a 13-week study. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**MODERATE: Hazard potential for developmental toxicity of the substituted amine phosphate mixture is estimated to be moderate based on data for piperazine moiety from piperazine phosphate and professional judgment. There is uncertainty if effects could occur at doses between 94 and 250 mg/kg/day because a LOAEL was not identified (the criteria cutoff dose for a LOW hazard designation is >250 mg/kg/day). Embryotoxicity was reported in conjunction with maternal toxicity and were considered to be secondary effects. Data for the substituted amine phosphate component showed no developmental effects in rats exposed during gestation to doses up to 1,060 mg/kg-day. A conservative approach was used since there were no measured values for the substituted amine phosphate mixture.**		
	Reproduction/ Developmental Toxicity Screen	**Piperazine:** Rabbit, oral; concern for developmental toxicity NOEL = 225 mg/kg/day	Professional judgment; Confidential study	Test substance identified as piperazine phosphate; a LOAEL was not identified. Reported in a confidential study.
		Piperazine: Rat, oral; concern for developmental toxicity NOEL = 1,000 mg/kg/day	Professional judgment; Confidential study	Test substance identified as piperazine phosphate; a LOAEL was not identified. Reported in a confidential study.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Prenatal Development	**Substituted amine phosphate component:** Signs of maternal toxicity at 136 mg/kg/day included decreased body weight and feed consumption, hematuria (23/25 rats), indrawn flanks (7/25 rats), and piloerection (1/25 rats). No adverse effects on gestational parameters and no signs of developmental toxicity were noted. NOAEL ≥1,060 mg/kg/day (Measured for the free base)	Confidential study	Reported in a confidential study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Piperazine: Rabbit, oral, GD 6-18. At 210 mg/kg/day piperazine base: maternal neurotoxicity, decreased body weight and food consumption; embryotoxic effects as resorption, retardation of ossification, and reduced fetal weight. These effects were considered secondary to maternal toxicity; no developmental effects or significant maternal toxicity was reported in the 94 mg/kg/day dose group. NOAEL (maternal toxicity) = 42 mg/kg/day piperazine base LOAEL (maternal toxicity) = 94 mg/kg/day piperazine base NOAEL (developmental) = 94 mg/kg/day piperazine base	ECHA, 2011	Reported in a secondary source. Test substance identified as piperazine phosphate; Developmental effects occurred at 210 mg/kg/day piperazine base; however, these effects occurred in conjunction with maternal toxicity and are considered secondary effects.
		Piperazine: Rat, oral, GD 6-15. At 210 mg/kg/day piperazine base: maternal toxicity: excessive salivation, lethargy and reduced body weight gain, body weight and food consumption at 2,100 mg/kg/day; No embyrotoxic effects reported. NOAEL (maternal toxicity) = 420 mg/kg/day piperazine base LOAEL (maternal toxicity) = 2100 mg/kg/day piperazine base NOAEL (developmental) = 2,100 mg/kg/day piperazine base	ECHA, 2011	Reported in a secondary source. Test substance identified as piperazine phosphate.
		Piperazine: Rabbit, oral; potential for developmental effects NOAEL = 225 mg/kg/day	Professional judgment	Estimated based on professional judgment.
	Postnatal Development			No data located.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Neurotoxicity		**LOW: Neurotoxicity hazard potential of the substituted amine phosphate mixture is estimated to be low based on expert judgment.**		
	Neurotoxicity Screening Battery (Adult)	Potential for neurotoxicity is expected to be low. (Estimated)	Expert judgment	Estimated based on expert judgment.
Repeated Dose Effects		**MODERATE: Repeated dose effects from the substituted amine phosphate mixture is estimated based on effects following repeated oral exposure to the substituted amine phosphate component in rats. Decreased body weight gain and feed consumption along with stones and diffuse epithelial hyperplasia in the urinary bladder were reported at a dose of 72 mg/kg/day. No data were located for the substituted amine phosphate mixture or salts.**		

Substituted Amine Phosphate Mixture			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Substituted amine phosphate component: Rat 28-day dietary toxicity study: Clinical signs included a dose-related increase in piloerection, lethargy, bloody urine spots in the cage and on the pelage of animals, and chromodacryorrhea. The incidence of urinary bladder calculi and urinary bladder hyperplasia in treated animals was dose-dependent, with a significant relationship between the calculi and hyperplasia. Calculi composition indicated the presence of an organic matrix containing the substituted amine phosphate component, phosphorus, sulfur, potassium, and chloride. Crystals of its monophosphate were identified in the urine. NOAEL: 2,000 ppm (240 mg/kg/day), excluding the observed increase in water consumption and the incidence of crystalluria LOAEL: 4,000 ppm (475 mg/kg/day) based on the formation of calculus (Measured for the free base)	Confidential study	Reported in a confidential study.

Substituted Amine Phosphate Mixture			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Substituted amine phosphate component: Rabbit and dog 28-day dietary toxicity study: No significant rise in the body temperature of rabbits was noted. Gross histological examination of the heart, lung, liver, spleen, thyroid, pancreas, intestines, kidneys and bladder did not show pathological changes. A zone of fat was found in the inner part of the renal cortex in 2 dogs, but also in the kidneys of 3 control dogs. (Measured for the free base)	Confidential study	Insufficient study details were reported in a confidential study. Unspecified number of animals tested.
	Substituted amine phosphate component: Rat 28-day dietary toxicity study: Incidence and size of bladder stones were directly related to the amount of substance administered. The larger stones were found to be unchanged in a matrix of protein, uric acid and phosphate. Lowest effective dose (LED): 1,500 ppm (~125 mg/kg) in males (Measured for the free base)	Confidential study	Insufficient study details were reported in a confidential study.

Substituted Amine Phosphate Mixture			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Substituted amine phosphate component: Rat 90-day dietary toxicity study: 1 male rat administered 18,000 ppm and 2 males administered 6,000 ppm died. Mean body weight gain and feed consumption were reduced. Stones and diffuse epithelial hyperplasia in the urinary bladders were observed in male rats of all treatment groups. Focal epithelial hyperplasia was observed in only 1 male. A second and third 13-week repeated dose toxicity study was conducted in rats at a dose range of 750 to 18,000 ppm bladder stones were observed at all dose levels. LOAEL: 750 ppm (72 mg/kg-day) based on urinary bladder stones (Measured for the free base)	Confidential study	Reported in a confidential study.

Substituted Amine Phosphate Mixture			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Substituted amine phosphate component: Mouse 90-day dietary toxicity study: A single female mouse died after receiving 9,000 ppm. Mean body weight gain relative to controls was depressed. The incidence of mice with bladder stones was dose-related and was greater in males than in females. 60% of mice having bladder ulcers also had urinary bladder stones. Bladder ulcers were multifocal or associated with inflammation (cystitis). Epithelial hyperplasia and bladder stones were observed together in 2 mice. Also, epithelial cell atypia was seen. NOAEL: 6,000 ppm (600 mg/kg-day) LOAEL: 9,000 ppm (900 mg/kg-day) (Measured for the free base)	Confidential study	Reported in a confidential study.
	Substituted amine phosphate component: Increased incidence of acute and chronic inflammation and epithelial hyperplasia of the urinary bladder was observed in mice following oral (feed) exposure for up to 103 weeks. There was also increased incidence of bladder stones in male mice. LOAEL = 2,250 mg/kg diet (lowest dose tested) (Measured for the free base)	Confidential study	Reported in a confidential study.; repeated dose effects described in a carcinogenicity bioassay study.
	Substituted amine phosphate component: Dog 1-Year dietary toxicity study: Crystalluria started 60 to 90 days into treatment and persisted during the study period. No other effects were observed.	Confidential study	Insufficient study details were reported in a confidential study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Substituted amine phosphate component: Rat 30-month dietary toxicity study: Neither accumulation of calculi nor any treatment-related urinary bladder lesions were found. (Measured for the free base)	Confidential study	Insufficient study details were reported in a confidential study.
		Substituted amine phosphate component: Rat 24 to 30-month dietary toxicity study: A dose-related trend for dilated glands in glandular gastric mucosa and inflammation in nonglandular gastric mucosa was observed. Urinary bladder calculi formation was not observed. (Measured for the free base)	Confidential study	Insufficient study details were reported in a confidential study.
		Piperazine: Rat 90-day dietary toxicity study: Only effect noted was a treatment-related decrease in body weight gain (>10%) NOAEL: 627 mg/kg-day LOAEL = 2394 mg/kg-day (Measured)	ECHA, 2011	According to guideline: FDA 1986, Toxicological principles for Safety Assessment of Direct Food Additives and Color Additives Used in Food; sufficient study details reported in a secondary source; dose recalculated to piperazine base (52,25% piperazine base).
Skin Sensitization		**MODERATE: Skin sensitization hazard potential for the substituted amine phosphate mixture is estimated to be moderate based on the piperazine component. Piperazine is a skin sensitizer in guinea pigs. Although the substituted amine phosphate component and an analog were not found to be skin sensitizers in guinea pigs, a conservative approach was used since there are no measured values for the substituted amine phosphate mixture.**		
	Skin Sensitization	**Substituted amine phosphate mixture:** No skin sensitization in guinea pigs using Magnusson-Kligman assay (Estimated by analogy)	Professional judgment; Confidential study	Based on closely related analogs with similar structures, functional groups, and physical/chemical properties.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Substituted amine phosphate component: No evidence of primary dermal irritation or sensitization in a human patch test. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: Non-sensitizing to guinea pigs. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Piperazine: Piperazine is a skin sensitizer in guinea pigs. Cross sensitization with other ethylene amines can also occur. (Measured)	ECHA, 2011	Study details reported in secondary source.
Respiratory Sensitization		**MODERATE: Respiratory sensitization hazard potential for the substituted amine phosphate mixture is estimated to be moderate based on analogy to the piperazine-containing compounds.**		
	Respiratory Sensitization	**Piperazine moiety:** Hazard potential for respiratory sensitization. (Estimated by analogy)	Professional judgment	Estimated based on analogy to piperazine-containing compounds.
Eye Irritation		**MODERATE: Eye irritation hazard due to the substituted amine phosphate mixture is estimated to be moderate based on data for a confidential analog showing eye irritation in rabbits. Although the substituted amine phosphate and piperazine components of the mixture are non-irritating to slightly irritating to rabbit eyes, a conservative approach was used since there are no measured values for the substituted amine phosphate mixture.**		
	Eye Irritation	**Substituted amine phosphate mixture:** moderate eye irritation in rabbits. (Estimated by analogy)	Professional judgment; Confidential studies	Reported in a confidential study. Based on two closely related analogs with similar structures, functional groups, and physical/ chemical properties.
		Substituted amine phosphate component: Non-irritating to rabbit eyes. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: Non-irritating to rabbit eyes following 0.5 mL of 10% solution. (Measured for the free base)	Confidential study	Limited study reported in a confidential study.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Substituted amine phosphate component: Mild irritant to rabbit eyes following exposure to 30 mg of dry powder. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: Slightly irritating to rabbit eyes. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Piperazine: Irritating to rabbit eyes. (Measured)	IUCLID, 2000	Results taken from 2 studies. Limited study details reported in a secondary source.
Dermal Irritation		**VERY HIGH: Dermal irritation hazard potential for the substituted amine phosphate mixture is estimated based on the piperazine component. Piperazine was corrosive to rabbit skin. Although the substituted amine phosphate component is not irritating to rabbit skin, a conservative approach was used since there are no measured values for the substituted amine phosphate mixture.**		
	Dermal Irritation	**Substituted amine phosphate mixture:** Not irritating to rabbit skin. (Estimated by analogy)	Professional judgment; Confidential study	Reported in a confidential study. Based on closely related analogs with similar structures, functional groups, and physical/chemical properties.
		Substituted amine phosphate component: Not irritating to rabbit skin. (Measured for the free base)	Confidential study	Reported in a confidential study; according to OECD 404 Guideline study.
		Substituted amine phosphate component: Not irritating to rabbit skin. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: Not irritating to rabbit skin. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Substituted amine phosphate component: Not irritating to rabbit skin. (Measured for the free base)	Confidential study	Limited study details reported in a confidential study.
		Piperazine: Not irritating to mild irritation to rabbit skin. (Measured)	IUCLID, 2000	Results taken from several studies. Limited study details reported In a secondary source.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Piperazine: Corrosive to rabbit skin. (category 2 – irritant) (Measured)	ECHA, 2011	Study details from two studies reported in secondary source; according to OECD Guideline 404.
Endocrine Activity		**There were insufficient data located to describe the effect of the substituted amine phosphate mixture on the endocrine system. In one study, the substituted amine phosphate component did not exhibit estrogenic activity *in vitro* in a yeast two-hybrid assay.**		
		Substituted amine phosphate component: Showed no estrogenic activity (no change in B-galactosidase activity) in an *in vitro* yeast two-hybrid assay in *Saccharomyces cerevisia* Y 190. (Measured for the free base)	Confidential study	Reported in a confidential study. No guideline followed.
Immunotoxicity		**There is estimated to be no potential for immunotoxicity of the substituted amine phosphate mixture based on expert judgment. Data located for the substituted amine phosphate component are not sufficient to determine the hazard potential for this endpoint.**		
	Immune System Effects	Potential for immunotoxicity is expected to be low. (Estimated)	Expert judgment	Estimated based on expert judgment.
		Substituted amine phosphate component: Did not inhibit the mitogenesis of B- and T- lymphocytes in an *in vitro* mouse lymphocyte mitogenesis test. (Measured for the free base)	Confidential study	Reported in a confidential study. Unclear how well mitogenesis test assesses immunotoxicity of chemicals.
ECOTOXICITY				
ECOSAR Class		Substituted amine phosphate component: Confidential structure class; Piperazine pyrophosphate: Aliphatic amines.		
Acute Toxicity		**MODERATE: Acute toxicity hazard for the substituted amine phosphate mixture is estimated based on an experimental LC_{50} value of 21 mg/L in *Daphnia magna* for the piperazine moiety of the ionized mixture which represents the most conservative value. Although measured toxicity values for the substituted amine phosphate free base indicate a low hazard designation for this component of the mixture, a conservative approach was used since there are no measured values for the substituted amine phosphate mixture.**		
Fish LC_{50}		**Substituted amine phosphate component:** *Leuciscus idus melanotus* 48-hour LC_{50} > 500 mg/L (Experimental)	Confidential study	Study details reported in a confidential study.

Substituted Amine Phosphate Mixture			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Substituted amine phosphate component: *Oryzias latipes* 48-hour LC_{50} = 1,000 mg/L (Experimental)	Confidential study	Study details reported in a confidential study.
	Substituted amine phosphate component: *Poecilia reticulata* 96-hour LC_{50} >3,000 mg/L (Experimental)	Confidential study	Study details reported in secondary source.
	Substituted amine phosphate component: *Poecilia reticulata* 4,400 mg/L dose lethal to <10% (Experimental)	Confidential study	Study details reported in a confidential study; unspecified exposure duration.
	Piperazine: *Poecilia reticulata* (guppy) 96-hour LC_{50} >1,800 mg/L Semi-static conditions (Experimental)	ECHA, 2011	Study details reported in a secondary source; according to EU Method C.1.
	Substituted amine phosphate component: Fish 96-hour LC_{50} = 391 mg/L (Estimated) ECOSAR: Confidential structure class	EPI	
	Substituted amine phosphate component: Fish 96-hour LC_{50} = 14,272 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Piperazine pyrophosphate: Fish 96-hour LC_{50} >10,000 mg/L (Estimated) ECOSAR: Aliphatic amines	EPI	No effects at saturation (NES): The LC_{50} value exceeds the water solubility ($1.0e^{+6}$ mg/L); NES are predicted for these endpoints.

Substituted Amine Phosphate Mixture			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Piperazine pyrophosphate: Fish 96-hour LC_{50} ≥10,000 mg/L (Estimated) ECOSAR: Neutral organics	EPI	NES: The LC_{50} value exceeds the water solubility ($1.0e^{+6}$ mg/L); NES are predicted for these endpoints.
Daphnid LC_{50}	**Substituted amine phosphate component:** *Daphnia magna* 48-hour LC_{50} >2,000 mg/L (Experimental)	Confidential study	Study details reported in a confidential study.
	Piperazine: *Daphnia magna* 48-hour LC_{50} = 21mg/L Static conditions (Experimental)	ECHA, 2011	Study details reported in a secondary source; according to EU Method C.2.
	Substituted amine phosphate component*:* Daphnid 48-hour LC_{50} = 144 mg/L (Estimated) ECOSAR: Confidential structure class	EPI	
	Substituted amine phosphate component: Daphnid 48-hour LC_{50} = 4,805 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Piperazine pyrophosphate: Daphnid 48-hour LC_{50} >10,000 mg/L (Estimated) ECOSAR: Aliphatic amines	EPI	
	Piperazine pyrophosphate: Daphnid 48-hour LC_{50} >10,000 mg/L (Estimated) ECOSAR: Neutral organics	EPI	NES: The LC_{50} value exceeds the water solubility ($1.0e^{+6}$ mg/L); NES are predicted for these endpoints.

Substituted Amine Phosphate Mixture			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Substituted amine phosphate component: *Scenedesmus pannonicus* 4-day EC_{50} = 940 mg/L (Experimental); 4-day NOEC = 320 mg/L (Experimental)	Confidential study	Reported in a confidential study.; Study details and test conditions were not provided.
	Substituted amine phosphate component: Green algae 96-hour EC_{50} = 325 mg/L (Estimated) ECOSAR: Confidential structure class	EPI	
	Substituted amine phosphate component: Green algae 96-hour EC_{50} = 4,396 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Piperazine pyrophosphate: Green algae 96-hour EC_{50} >10,000 mg/L (Estimated) ECOSAR: Aliphatic amines	EPI	
	Piperazine pyrophosphate: Green algae 96-hour EC_{50} >10,000 mg/L (Estimated) ECOSAR: Neutral organics	EPI	NES: The LC_{50} value exceeds the water solubility ($1.0e^{+6}$ mg/L); NES are predicted for these endpoints.
Chronic Aquatic Toxicity	**LOW: The substituted amine phosphate mixture chronic toxicity hazard potential is estimated based on measured chronic toxicity values for the piperazine moiety, on estimated values for piperazine pyrophosphate, and on estimated values for the substituted amine phosphate component of the mixture, for all three surrogate species.**		
Fish ChV	**Substituted amine phosphate component:** *Jordanella floridae* 35-day NOEC ≥1,000 mg/L (Experimental)	Confidential study	Reported in a confidential study; study details and test conditions were not provided.

Substituted Amine Phosphate Mixture			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Substituted amine phosphate component: *Salmo gairdneri* NOEC (macroscopic) = 500 mg/L (Experimental); NOEC (microscopic) <125 mg/L (Experimental)	Confidential study	Reported in a confidential study; study details and test conditions were not provided.
	Substituted amine phosphate component: *Daphnia magna* 21-day LC_{50} = 32-56 mg/L, 21-day LC_{100} = 56 mg/L, 21day NOEC = 18 mg/L (Experimental)	Confidential study	Reported in a confidential study; study details and test conditions were not provided.
	Substituted amine phosphate component: Fish ChV = 1,102 mg/L (Estimated) ECOSAR: Confidential structure class	EPI	
	Substituted amine phosphate component: Fish ChV = 1,076 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Piperazine pyrophosphate: Fish ChV ≥10,000 mg/L (Estimated) ECOSAR: Aliphatic amines	EPI	
	Piperazine pyrophosphate: Fish ChV ≥10,000 mg/L (Estimated) ECOSAR: Neutral organics	EPI	NES: The LC_{50} value exceeds the water solubility ($1.0e^{+6}$ mg/L); NES are predicted for these endpoints.

Substituted Amine Phosphate Mixture			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Daphnid ChV	**Piperazine:** *Daphnia magna* 21-day NOEC = 12.5 mg/L (immobile neonates) LOEC = 25 mg/L (immobile neonates) NOEC = 50 mg/L (reproduction) NOEC = 25 mg/L (growth) Semi-static conditions (Experimental)	ECHA, 2011	Study details reported in a secondary source; according to OECD Guideline 211.
	Substituted amine phosphate component: Daphnid ChV = 14.85 mg/L (Estimated) ECOSAR: Confidential structure class	EPI	The toxicity value was estimated through application of acute-to-chronic ratios
	Substituted amine phosphate component: Daphnid ChV = 343.93 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Piperazine pyrophosphate: Daphnid ChV = 2,408 mg/L (Estimated) ECOSAR class: Aliphatic amines	EPI	
	Piperazine pyrophosphate: Daphnid ChV >10,000 mg/L (Estimated) ECOSAR: Neutral organics	EPI	NES: The LC_{50} value exceeds the water solubility ($1.0x10^6$ mg/L); NES are predicted for these endpoints.
Green Algae ChV	**Piperazine:** *Selenastrum capricornutum (Pseudokirchnerella subcapitata)* 72-hour NOEC >1,000 mg/L (growth rate) Static conditions (Experimental)	ECHA, 2011	Study details reported in secondary source; according to OECD Guideline 201.

Substituted Amine Phosphate Mixture			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Substituted amine phosphate component: Green algae ChV = 0.70 mg/L (Estimated) ECOSAR: Confidential structure class	EPI	The toxicity value was estimated through application of acute-to-chronic ratios.
	Substituted amine phosphate component: Green algae ChV = 81.26 mg/L (Estimated) ECOSAR: Confidential structure class	EPI	The toxicity value was estimated through application of acute-to-chronic ratios.
	Substituted amine phosphate component: Green algae ChV = 313.17 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Piperazine pyrophosphate: Green algae ChV >10,000 mg/L (Estimated) ECOSAR: Aliphatic amines	EPI	
	Piperazine pyrophosphate: Green algae ChV = 259,000 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
ENVIRONMENTAL FATE			
Transport	**The substituted amine phosphate mixture is comprised of approximately 50% piperazine pyrophosphate and 50% of a substituted amine phosphate. Both of these ionic compounds have high estimated water solubility. Therefore, this mixture can be expected to partition predominately to water and soil. The components are anticipated to migrate from soil into groundwater based on the estimated K_{oc} values of <100. Volatilization from either wet or dry surfaces is not expected to be an important fate process based on the estimated vapor pressure of this mixture.**		

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment	In water, the substituted amine phosphate mixture components are expected to be fully dissociated. Volatilization of the dissociated species from either wet surfaces is not expected to be an important fate process.
		Piperazine pyrophosphate: $<10^{-10}$ (Estimated)	EPI	
		Substituted amine phosphate: $<10^{-10}$ (Estimated)	EPI	
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	**Piperazine pyrophosphate:** 62 (Estimated)	EPI	
		Substituted amine phosphate: 13 (Estimated)	EPI	
	Level III Fugacity Model	**Piperazine pyrophosphate:** Air = <1% (Estimated) Water = 20% Soil = 80% Sediment = <1%	EPI	
		Substituted amine phosphate: Air = <1% (Estimated) Water = 35% Soil = 65% Sediment = <1%	EPI	
Persistence		**HIGH: The substituted amine phosphate mixture is estimated to show high persistence in the environment based on experimental data for the dissociation species of the substituted amine phosphate component and piperazine pyrophosphate. Additionally, biodegradation estimates for piperazine pyrophosphate and the substituted amine phosphate component suggest high persistence for these ionic compounds.**		

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Water	**Aerobic Biodegradation**	**Piperazine pyrophosphate:** Days-Weeks (Primary survey model) Weeks-Months (Ultimate survey model)	EPI	
		Piperazine: Not readily biodegradable according to OECD 301C; 1.4% degradation after 2 weeks. (Measured for free base)	MITI, 1998	Measured biodegradation indicate slow removal by this pathway for the dissociated species, piperazine.
		Piperazine: Readily biodegradable according to OECD 301F; 65-70% in 2 weeks by O_2 and CO_2 and 39% by dissolved organic carbon (DOC) and OECD 301D; 90% in 2 weeks. Inherently biodegradable according to 302A; 96% degradation after 52 days. (Measured for free base)	ECHA, 2011	Measured biodegradation indicate potential for biodegradation for the dissociated species, piperazine.
		Substituted amine phosphate: Weeks (Primary survey model) Months (Ultimate survey model)	EPI	
		Substituted amine phosphate dissociation product: The range of reported aerobic biodegradation rates span from 0% removal to <30% removal after 14 days with activated sludge. (Measured for dissociation species)	Confidential study	Measured biodegradation indicate limited removal by this pathway for a dissociated species of the substituted amine phosphate.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the estimated Henry's Law Constant and the low rates of volatilization for completely dissociated species; applies to both ionic solids present in the substituted amine phosphate mixture.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the estimated Henry's Law Constant and the low rates of volatilization for completely dissociated species; applies to both ionic solids present in the substituted amine phosphate mixture.
Soil	**Aerobic Biodegradation**	**Substituted amine phosphate dissociation product:** Not readily biodegradable: 0% biodegradation detected after 2 weeks with 100 ppm in 30 ppm activated sludge (OECD TG 301C) (Measured); 0% degradation after 28 days with 100 mg DOC/L in activated sludge (Zahn-Wellens test, OECD 302B) (Measured) **Piperazine*:*** In a variety of soil samples, complete degradation took 24 to 68 days with a lag period of 15 to 60 days respectively. Some samples reported no degradation at 3 months. (Measured for free base)	Confidential study; EU RAR, 2005	Value for dissociation product of the substituted amine phosphate component and piperazine pyrophosphate dissociation species, piperazine. Measured biodegradation demonstrate removal by this pathway.
	Anaerobic Biodegradation	**Substituted amine phosphate dissociation product:** 0-8.9% nitrification was observed after 28 days incubation with bacteria in Webster silty clay loam under anaerobic conditions (Measured) **Piperazine*:*** No degradation after 6 months under denitrifying, sulfate reducing, or methanogenic conditions. (Measured for free base)	Confidential study; Bae, 2002	Value for dissociated component of the substituted amine phosphate and piperazine pyrophosphate dissociation species, piperazine. Measured biodegradation rates demonstrate no removal by this pathway.

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Soil Biodegradation with Product Identification	**Substituted amine phosphate dissociation product:** Nitrification occurs in soil at a low rate (0.7 % organic N found as NO_3-N in week 10, and 0 % in week 28). (Measured)	Confidential study	Nonguideline study for the dissociated product of the substituted amine phosphate component.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.
Reactivity	**Photolysis**	**Substituted amine phosphate:** Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	This compound does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths.
		Piperazine: 0.8 hour half-life (Measured for free base)	OECD SIDS, 2004	Value for piperazine pyrophosphate dissociation species, piperazine.
	Hydrolysis	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	Both ionic solids present in the substituted amine phosphate mixture do not contain functional groups that would be expected to hydrolyze readily under environmental conditions.
Environmental Half-Life		**Substituted amine phosphate:** 120 days	EPI; PBT Profiler	Half-life estimated for the predominant compartment, as determined by EPI and the PBT Profiler methodology.
		Piperazine pyrophosphate: 75 days	EPI; PBT Profiler	
Bioaccumulation		**LOW: The substituted amine phosphate mixture is expected to have low potential for bioconcentration and bioaccumulation based on an estimated BCF and BAF values of <100 for the two components of the mixture, piperazine pyrophosphate and substituted amine phosphate.**		

Substituted Amine Phosphate Mixture				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Fish BCF	**Piperazine pyrophosphate:** 3.2 (Estimated)	EPI	
		Substituted amine phosphate component: 3.2 (Estimated)	EPI	
	BAF	**Piperazine pyrophosphate:** 0.9 (Estimated)	EPI	
		Substituted amine phosphate component: 0.9 (Estimated)	EPI	
	Metabolism in Fish	**Substituted amine phosphate dissociation product:** Uptake, bioaccumulation and elimination study with ^{14}C-labeled compound in fathead minnow (BCF = 0.48 and 0.26) and rainbow trout (BCF = 0.11, 0.05, 0.03) (Measured)	Confidential study	Nonguideline study that supports the low bioaccumulation concern for this substance and its dissociation products.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		These chemicals were not included in the NHANES biomonitoring report (CDC, 2011).		

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Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether

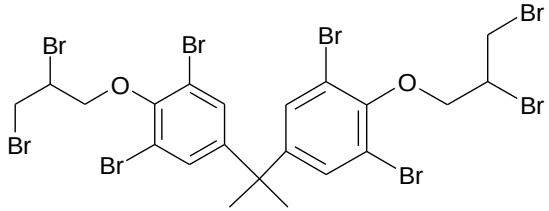
Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether	21850-44-2	L	*M*	M	*M*	*M*	*L*	*M*	*M*		*L*	*L*	*L*	*L*	VH	*H*

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether



CASRN: 21850-44-2

MW: 943.62

MF: $C_{21}H_{20}Br_8O_2$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: O(c1c(cc(cc1Br)C(c1cc(c(OCC(Br)CBr)c(c1)Br)Br)(C)C)Br)CC(Br)CBr

Synonyms: Benzene, 1,1'-(1-methylethylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)- (TSCA Inventory); 1,1'-(1-Methylethylidene)bis(3,5-dibromo-4-(2,3-dibromopropoxy))benzene; 1,1'-(1-Methylethylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)]benzene; 1,1'-(Isopropylidene)bis(3,5-dibromo-4-(2,3-dibromopropoxy)benzene); 1,1'-(isopropylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)benzene]; 1,1'-propane-2,2-diylbis[3,5-dibromo-4-(2,3-dibromopropoxy)benzene]; 2,2-Bis[3,5-dibromo-4(2,3-dibromopropoxy)phenyl]propane; 2,2-Bis[3,5-dibromo-4-(2,3-dibromopropyloxy)phenyl]propane; 2,2-Bis[4-(2,3-dibromopropoxy)-3,5-dibromophenyl]propane; 3,3’,5,5’-TetrabromobisphenolA bis92,3-dibromopropyl) ether; 4,4’-Isopropylidenebis[2,6-dibromo-1-(2,3-dibromopropoxy)benzene]; 403AF; Bis(2,3-dibromopropoxy)tetrabromobisphenol A; Bromcal 66.8; Bromkal 66-8; D 5532; Dibromopropydian; FG 3100; FR 720; Fire guard 3100; Flame Cut 121K; Flame Cut 121R; GX 5532; Propane, 2,2-bis[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]-; PE-68; Pyroguard SR 720; SR 720; SAYTEX HP-800 A, HP-800 AG, HP-800 AGC; Tetrabromobisphenol A bis(2,3-dibromopropyl ether); Tetrabromobisphenol A bis(2,3-dibromopropyl) ether; Tetrabromobisphenol-A-bis-2,3-dibromopropyl ether Tetrabromobisphenol-A-bis-2,3-dibromopropylether;

Chemical Considerations: This is a discrete organic chemical with a MW below 1,000. EPI v 4.0 was used to estimate physical/chemical and environmental fate values as required. Measured values for available endpoints were incorporated into the estimations.

Polymeric: No
Oligomers: Not applicable

Metabolites, Degradates and Transformation Products: TBBPA bis(bromopropenyl ether) and TBBPA.

Analog: No analog
Endpoint(s) using analog values: Not applicable

Analog Structure: Not applicable

Structural Alerts: Polyhalogenated aromatic hydrocarbons, immunotoxicity (U.S. EPA, 2011a)

Risk Phrases: Not classified by Annex I Directive 67/548/EEC & IUCLID (Pakalin et al., 2007).

Hazard and Risk Assessments: Risk assessment complete for TBBPA bis (2,3-dibromopropyl) ether by the European Chemicals Bureau in 2007 (Pakalin et al., 2007).

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory and is subject to a Section 4 test rule.

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether CASRN 21850-44-2			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	117 (Measured)	Tokyo Chemical Industry Co., 2010; ChemSpider, 2011	Selected value for assessment.
	114 (Measured)	NICNAS, 2001	Sufficient details were not available to assess the quality of this study; value reported in a secondary source.
	90-100 (Measured)	IPCS, 1995; Great Lakes Chemical Corporation, 1982a	These reported values may be for a commercial mixture.
	95 (Measured)	Mack, 2004	
Boiling Point (°C)	Decomposition at >270 (Measured)	IPCS, 1995	Decomposition is expected before the boiling point is reached.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	EPI; EPA, 2011b	Cutoff value for non volatile compounds according to SF assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	EPI; EPA, 1999	Cutoff value for non soluble compounds according to HPV assessment guidance.
	1×10^{3} (Measured)	IPCS, 1995	Inadequate; these values are not consistent with a non polar, highly brominated material with a MW near 1,000.
	$<1\times10^{3}$ (Measured)	NICNAS, 2001	
Log K_{ow}	>10 (Estimated)	EPI; EPA, 2011b	Cutoff value used according to SF assessment guidance.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether CASRN 21850-44-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
pK_a		Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**TBBPA bis (2,3-dibromopropyl) ether, as a neat material, is estimated not to be absorbed through the skin, to have poor skin absorption when in solution, and to have poor absorption via the lungs and gastrointestinal tract. An experimental study in rats showed that the majority (95%) of TBBPA bis (2,3-dibromopropyl) ether is rapidly eliminated in the feces following single or multiple oral doses and absorption is slow and minimal. However, if absorbed, TBBPA bis (2,3-dibromopropyl) ether is slowly eliminated from the blood, with the liver being the main organ for deposition.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	Not absorbed through the skin as a neat material and poor absorption through skin when in solution; poor absorption through the lung and gastrointestinal tract. (Estimated by analogy)	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/chemical properties.

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether CASRN 21850-44-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Following single or repeated (5 or 10 days) oral administrations of 20 mg/kg [^{14}C]-TBBPA bis (2,3-dibromopropyl) ether to male F-344 rats, the compound was poorly absorbed from the gastrointestinal tract and uptake to the systemic circulation was considered slow. The C_{max} (0.6 µg/mL) occurred at 7.4 hours after dosing. Distribution to the tissues accounted for < 1% of the dose at 96 hours while 95% of the dose (in [^{14}C] equivalents) was excreted in the feces within 36 hours of administration. Elimination in the urine accounted for <0.1% of the administered dose and 1% of the dose (as metabolites) was excreted in the bile after 24 hours.	Knudsen et al., 2007	Study details reported in primary source.
Acute Mammalian Toxicity		**LOW: Based on oral and dermal LD_{50} values >2, 000 mg/kg and an inhalation LC_{50} value >20 mg/L.**		
Acute Lethality	**Oral**	Mouse LD_{50} >20,000 mg/kg	IPCS, 1995	Limited study details reported in a secondary source.
	Dermal	Mouse LD_{50} >20,000 mg/kg	IPCS, 1995	Limited study details reported in a secondary source.
	Inhalation	Mouse LC_{50} >87,000 mg/m^3 (87 mg/L)	Great Lakes Chemical Corporation, 1982b	Limited study details reported in a secondary source.
Carcinogenicity		**MODERATE: No data located. Estimated to have potential for carcinogenicity based on the potential for alkylation and professional judgment.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)	There is potential for carcinogenicity effects based on a mechanistic consideration of the potential for alkylation (Estimated)	Professional judgment	Based on mechanistic considerations.

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether CASRN 21850-44-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Combined Chronic Toxicity/ Carcinogenicity			No data located.
Genotoxicity		**MODERATE: TBBPA bis (2,3-dibromopropyl) ether was mutagenic to *Salomonella typhimurium* but did not cause chromosomal aberrations in CHO cells (*in vitro*), was negative in an *in vivo* micronucleus assay in mice and did not produce unscheduled DNA synthesis in rats. TBBPA bis (2,3-dibromopropyl) ether is also estimated to have potential for genotoxicity based on the potential for alkylation.**		
	Gene Mutation *in vitro*	There is potential for mutagenicity based on a mechanistic consideration of the potential for alkylation (Estimated)	Professional judgment	Based on closely related confidential analogs with similar structures and functional groups.
		Positive, Ames assay (standard plate) in *Salmonella typhimurium* strains TA1535 and TA100 with and without metabolic activation and TA98 without metabolic activation.	Great Lakes Chemical Corporation, 1982a	Sufficient study details reported.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	Negative chromosomal aberrations in CHO cytogenetic assay with and without metabolic activation (precipitation was observed at the highest concentration).	IPCS, 1995	Reported in a secondary source.
	Chromosomal Aberrations *in vivo*	Negative for micronuleated polychromatic erythrocytes in B6C3F1 mice.	NTP, 2011	Reported in a secondary source.
	DNA Damage and Repair	Negative for unscheduled DNA synthesis assay in Sprague Dawley rats at 10, 50, 100, 500 or 1,000 µg/mL.	IPCS, 1995	Reported in a secondary source.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**MODERATE: Estimated to have potential for reproductive effects based on the potential for alkylation and professional judgment.**		

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether CASRN 21850-44-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Reproduction/ Developmental Toxicity Screen	There is potential for reproductive effects based on a mechanistic consideration of the potential for alkylation (Estimated)	Professional judgment	Based on mechanistic considerations.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Reproduction and Fertility Effects			No data located.
Developmental Effects		**MODERATE: Estimated to have potential for developmental effects based on the potential for alkylation and professional judgment.**		
	Reproduction/ Developmental Toxicity Screen	There is potential for developmental effects based on a mechanistic consideration of the potential for alkylation (Estimated)	Professional judgment	Based on mechanistic considerations.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Prenatal Development			No data located.
	Postnatal Development			No data located.
Neurotoxicity		**LOW: Estimated not to have potential for neurotoxicity based on expert judgment; no data located.**		
	Neurotoxicity Screening Battery (Adult)	Low potential for neurotoxicity. (Estimated)	Expert judgment	Estimated based on expert judgment.
Repeated Dose Effects		**MODERATE: There is potential for liver toxicity because TBBPA bis (2,3-dibromopropyl) ether is a highly brominated compound. Located data were insufficient.**		

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether CASRN 21850-44-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Potential for liver effects based on a mechanistic consideration of this highly brominated compound (Estimated)	Professional judgment	Based on closely related confidential analogs with similar structures and functional groups.
		Mice were administered TBBPA bis (2,3-dibromopropyl) ether in their diet at 200 or 2,000 mg/kg-day for 90 days. No deaths, or abnormal symptoms observed in gross pathological examination.	IPCS, 1995	Limited study details reported in a secondary source.
Skin Sensitization		**MODERATE: No data located. Estimated to have potential for skin sensitization based on the potential for alkylation and professional judgment.**		
	Skin Sensitization	There is potential for skin sensitization based on a mechanistic consideration of the potential for alkylation. (Estimated by analogy)	Professional judgment	Based on mechanistic considerations.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Estimated to not cause eye irritation based on expert judgment.**		
	Eye Irritation	Low potential for eye irritation. (Estimated)	Expert judgment	Estimated based on expert judgment.
		Workers report development of eye irritation following exposure to a complex mixture of airborne contaminants that included TBBPA bis (2,3-dibromopropyl) ether.	Great Lakes Chemical Corporation, 1999	Evidence is based on isolated incidents and workers were exposed to a complex mixture of airborne contaminants while melt processing that uses thermoplastic resin formulators containing this substance as an additive.
Dermal Irritation		**LOW: Estimated to not cause dermal irritation based on expert judgment.**		
	Dermal Irritation	Low potential for dermal irritation. (Estimated)	Expert judgment	Estimated based on expert judgment.

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether CASRN 21850-44-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Workers report development of dermal irritation following exposure to a complex mixture of airborne contaminants that included TBBPA bis (2,3-dibromopropyl) ether.	Great Lakes Chemical Corporation, 1999	Evidence is based on isolated incidents and workers were exposed to a complex mixture of airborne contaminants while melt processing that uses thermoplastic resin formulators containing this substance as an additive.
Endocrine Activity		**Based on 4 *in vitro* assays, TBBPA bis (2,3-dibromopropyl) ether can interact with the endocrine system. TBBPA bis (2,3-dibromopropyl) ether may have potential estrogenic and transthyretin-binding effects. TBBPA bis (2,3-dibromopropyl) ether appears to inhibit sulfation of estradiol (E2), but does not exhibit estrogenic activity via interference with estrogen receptors (ER). TBBPA bis (2,3-dibromopropyl) ether also does not appear to interfere with AhR -mediated, androgenic or progestagenic pathways. TBBPA bis (2,3-dibromopropyl) ether competed with thyroid hormone precursor thyroxine (T4) for binding to human transthyretin (TTR), but did not exhibit thyroid hormone (T3) mimicking activity.**		
		Negative; did not cause inhibition of CYP17 catalytic activity in human H295R adrenocortical carcinoma cells.	Cantón et al., 2006	Data taken from primary study.
		Positive for estradiol sulfotransferase (E2SULT)-enzyme inhibition in E2SULT assay	Hamers et al., 2006	Data taken from primary study.
		Negative for agonistic and antiagonistic interactions with aryl hydrocarbon (AhR), androgen (AR), progesterone (PR), and estrogen (ER) receptors in series of CALUX assays.	Hamers et al., 2006	Data taken from primary study.
		Positive for displacement of thyroid hormone precursor thyroxine (T4) from plasma transport protein in TTR binding assay	Hamers et al., 2006	Data taken from primary study.
		Negative for potentiating and antagonistic activity with T3-mediated cell proliferation in T-screen.	Hamers et al., 2006	Data taken from primary study.

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether CASRN 21850-44-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Immunotoxicity		**Potential for immunotoxicity based on the presence of the polyhalogenated aromatic hydrocarbons structural alert and professional judgment.**		
	Immune System Effects	Potential for immunotoxicity based on the presence of the polyhalogenated aromatic hydrocarbons structural alert.	EPA, 2011a; Professional judgment	Estimated based on the presence of a structural alert
ECOTOXICITY				
ECOSAR Class		Halo ethers, Neutral organics		
Acute Toxicity		**LOW: Based on estimated acute toxicity values for fish, daphnid, and algae that suggest no effects at saturation (NES).**		
Fish LC_{50}		Fish 96-hour LC_{50} = 0.00101 mg/L ECOSAR: Halo ethers	EPI	NES: The log K_{ow} of 11.52 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted.
		Fish 96-hour LC_{50} = $6.44x10^{-6}$ mg/L ECOSAR: Neutral organics	EPI	NES: The log K_{ow} of 11.52 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted.
Daphnid LC_{50}		Daphnia 48-hour LC_{50} = 0.000637 mg/L ECOSAR: Halo ethers	EPI	NES: The log K_{ow} of 11.52 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted.
		Daphnia 48-hour LC_{50} = $0.1.17x10^{-5}$ mg/L ECOSAR: Neutral organics	EPI	NES: The log K_{ow} of 11.52 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0; NES are predicted.
Green Algae EC_{50}		Green algae 96-hour EC_{50} = 0.000251 mg/L ECOSAR: Neutral organics	EPI	NES: The log K_{ow} of 11.52 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4; NES are predicted.
Chronic Aquatic Toxicity		**LOW: Based on estimated chronic toxicity values for fish, daphnid and green algae that suggest NES.**		
Fish ChV		Fish ChV = $1.33x10^{-6}$ mg/L ECOSAR: Halo ethers	EPI	NES: The log K_{ow} of 11.52 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted.
		Fish ChV = $4.95x10^{-7}$ mg/L ECOSAR: Neutral organics	EPI	NES: The log K_{ow} of 11.52 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted.

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether CASRN 21850-44-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Daphnid ChV		Daphnid ChV = 1.93×10^{-5} mg/L ECOSAR: Halo ethers	EPI	NES: The log K_{ow} of 11.52 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted.
		Daphnid ChV = 5.83×10^{-6} mg/L ECOSAR: Neutral organics	EPI	NES: The log K_{ow} of 11.52 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted.
Green Algae ChV		Green Algae ChV = 0.000517 mg/L ECOSAR: Neutral organics	EPI	NES: The log K_{ow} of 11.52 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0; NES are predicted.
ENVIRONMENTAL FATE				
Transport		**Evaluation of TBBPA bis (2,3-dibromopropyl) ether transport is based entirely on estimations from quantitative structure-activity relationships (QSARs). TBBPA bis (2,3-dibromopropyl) ether is expected to have low mobility in soil based on estimations indicating strong absorption to soil. If released to the atmosphere, TBBPA bis (2,3-dibromopropyl) ether is likely to exist solely as particulate. As a particulate, atmospheric oxidation is not expected to be a significant route of environmental removal. Based on the Henry's Law Constant, volatilization from water or moist soil is not expected to occur at an appreciable rate. Level III fugacity models indicate that TBBPA bis (2,3-dibromopropyl) ether will partition predominantly to sediment and soil.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	EPI; Professional judgment	Cutoff value for non volatile compounds.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	EPI; EPA, 2011b	Cutoff value for non mobile compounds according to SF assessment guidance.
	Level III Fugacity Model	Air = <1% (Estimated) Water = 5% Soil = 95% Sediment = <1%	EPI	

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether CASRN 21850-44-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Persistence		**VERY HIGH: High persistence of TBBPA bis (2,3-dibromopropyl) ether is expected as a result of located biodegradation studies and the absence of other expected likely removal processes under environmental conditions. In the course of a 28-day MITI test, only 1% of TBBPA bis (2,3-dibromopropyl) ether was degraded. TBBPA bis (2,3-dibromopropyl) ether will exist primarily in the particulate phase in the atmosphere and is not expected to undergo removal by gas phase oxidation reactions. It is also not anticipated to undergo removal by hydrolysis.**		
Water	**Aerobic Biodegradation**	1% after 4 weeks OECD 301C; test concentration of 100 mg/L and concentration of activated sludge inoculum of 30 mg/L (Measured)	MITI, 2007	Adequate, guideline study.
	Volatilization Half-life for Model River	>1 year (Estimated)	EPI	
	Volatilization Half-life for Model Lake	>1 year (Estimated)	EPI	
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation	Not probable (Estimated)	Professional judgment	Large MW substances are not anticipated to be assimilated by microorganisms. Therefore, anaerobic biodegradation is not expected to be an important removal process.
	Soil Biodegradation w/ Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	12 hours (Estimated)	EPI	
Reactivity	**Photolysis**			No data located.
	Hydrolysis	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to hydrolyze readily under environmental conditions.

Tetrabromobisphenol A Bis (2,3-dibromopropyl) Ether CASRN 21850-44-2				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Environmental Half-life		>180 days (Estimated)	EPI; PBT Profiler	Half-life estimated for the predominant compartment, as determined by EPI and the PBT Profiler methodology.
Bioaccumulation		**HIGH: Based on an estimated BAF of 12,000 and its detection in Great Lakes Herring gull eggs, potential for bioaccumulation is high.**		
	Fish BCF	3.4 to 43 (15 µg/L concentration) <17 to 130 (1.5 µg/L concentration) (Measured)	MITI, 2007	Adequate, guideline study.
	BAF	12,000 (Estimated)	EPI	
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		TBBPA bis (2,3-dibromopropyl) ether was identified in dust collected near an artificial stream and pond system in Berlin, Germany (Harju et al., 2009); in sewage sludge samples from southern China; in sediments from southern China (Shi et al., 2009) and in water, sediment and soil along the Liuyang River in China (Qu et al., 2011).		
Ecological Biomonitoring		Detected in Great Lakes Herring gull eggs (Letcher and Chu, 2010).		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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TBBPA Glycidyl Ether, TBBPA Polymer

Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

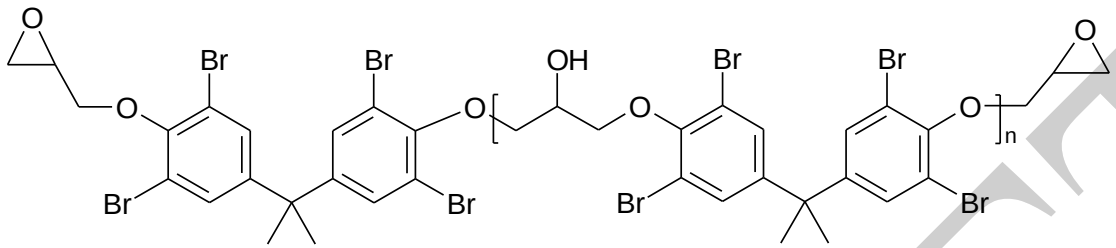
VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH)* were assigned using values from estimation software and professional judgment.

[d] This hazard designation is driven by potential for lung overloading as a result of dust forming operations.

♦ Different formulations of the commercial product are available. One of these many formulations has an average MW of ~1,600 and contains significant amounts of lower MW components. These lower MW components are primarily unchanged starting materials that have hazard potentials different than the polymeric flame retardant, as follows: VERY HIGH- Estimated potential for bioaccumulation; HIGH-Experimental concern for acute aquatic toxicity; HIGH-Estimated potential for chronic aquatic toxicity; MODERATE-Experimental concern for developmental; and MODERATE-Estimated potential for carcinogencity, genotoxicity, repeated dose, reproductive, and skin and respiratory sensitization toxicity.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
TBBPA Glycidyl Ether, TBBPA Polymer	68928-70-1	*L*	*L*♦	*L*♦	*L*♦	*L*♦	*L*	*M*♦ [d]	*L*♦	♦	*L*	*L*	*L*♦	*L*♦	*VH*	*L*♦

TBBPA Glycidyl Ether, TBBPA Polymer



CASRN: 68928-70-1

MW: 10,000 to >50,000; 0% <1,000

MF: $(C_{21}H_{20}Br_4O_4 \cdot C_{15}H_{12}Br_4O_2)_n$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: The polymer component with MW >1,000 is not amenable to SMILES notation.

Synonyms: Phenol, 4,4'-(1-methylethylidene)bis[2,6-dibromo-, polymer with 2,2'-[(1-methylethylidene)bis[(2,6-dibromo-4,1-phenylene)oxymethylene]]bis[oxirane] (TSCA Inventory); 4,4'-propane-2,2-diylbis(2,6-dibromophenol) - 2,2'-{propane-2,2-diylbis[(2,6-dibromobenzene-4,1-diyl)oxymethanediyl]}dioxirane (1:1); Tetrabromobisphenol A - Tetrabromobisphenol A diglycidyl ether polymer; Tetrabromobisphenol A, 2,2-bis(4-(2,3-epoxypropyloxy)dibromophenyl)propane polymer

Chemical Considerations: This alternative is a high MW polymer. The extent of polymerization and thus average MW is formulation dependent. The higher MW oligomers, with a MW >1,000, are assessed together using the Sustainable Futures (SF) polymer assessment criteria in this report (U.S. EPA, 2010). However, it should be noted that at least one formulation of CASRN 68928-70-1 has a number average molecular weight (MW_n) of 1,600 with 12.7% <1,000 resulting from the presence of unchanged starting materials. The summary of the hazards of these unchanged starting materials, if present in the commercial formulation, are provided in Table 4-4 as a footnote (♦).

Polymeric: Yes
Oligomers: Commercial brominated epoxy polymer products represented by CASRN 68928-70-1 typically are comprised of high MW epoxy-terminated oligomers.

Metabolites, Degradates and Transformation Products: None

Analog: No analog
Endpoint(s) using analog values: Not applicable

Analog Structure: Not applicable

Structural Alerts: None identified

Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).

Hazard and Risk Assessments: None identified

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory and is exempt from reporting under the Chemical Data Reporting rule (CDR).

TBBPA Glycidyl Ether, TBBPA Polymer CASRN 68928-70-1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	135–150 (Measured)	ICL Industrial Products, 2011	For the commercial product F-2300H. The melting points reported cover a broad range and are anticipated to be formulation specific liquid-glass transition temperatures.
	105-115; 150 ± 5 (Measured)	NICNAS, 2001	For the commercial product F-2300H. The melting points reported cover a broad range and are anticipated to be formulation specific liquid-glass transition temperatures.
Boiling Point (°C)	>300 (Estimated)	Professional judgment	Cutoff value used for large, high MW solids.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW non-ionic polymers according to SF polymer assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW non-ionic polymers according to SF polymer assessment guidance.
	Insoluble (Measured)	ICL Industrial Products, 2011; NICNAS, 2001	For the commercial product F-2300H; qualitative value that cannot be used to evaluate other endpoints within the hazard assessment.
Log K_{ow}			No data located; polymers with a MW >1,000 are outside the domain of the available estimation methods.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.

TBBPA Glycidyl Ether, TBBPA Polymer CASRN 68928-70-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
pH		Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a		Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**There is no absorption expected for any route of exposure. This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is not expected to be readily absorbed, distributed or metabolized in the body. However, there are formulations of the commercial product available that may contain significant amounts of lower MW components; absorption may occur more readily in this case.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral**	No absorption is expected for any route of exposure (Estimated)	Professional judgment	Estimated based on professional judgment.
Acute Mammalian Toxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore is of low potential for acute mammalian toxicity.**		
Acute Lethality	**Oral** **Dermal** **Inhalation**	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
Carcinogenicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have few to no residual monomers, crosslinking, swellability, dispersability, potential for inhalation, nor hindered amine groups and therefore has low potential for carcinogenicity.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse) **Combined Chronic Toxicity/ Carcinogenicity**	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.

TBBPA Glycidyl Ether, TBBPA Polymer CASRN 68928-70-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Genotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for genotoxicity.**		
	Gene Mutation *in vitro*	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Gene Mutation *in vivo*			
	Chromosomal Aberrations *in vitro*			
	Chromosomal Aberrations *in vivo*			
	DNA Damage and Repair			
	Other (Mitotic Gene Conversion)			
Reproductive Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for reproductive effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			
Developmental Effects		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for developmental effects.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2010	Based on SF polymer assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			

TBBPA Glycidyl Ether, TBBPA Polymer CASRN 68928-70-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Postnatal Development			
Neurotoxicity		**LOW: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for neurotoxicity.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
Repeated Dose Effects		**MODERATE: This polymer is large, with a MW >1,000. It is expected to have limited bioavailability; however, because the MW_n is >10,000 there is the possibility of lung overloading in dust forming conditions.**		
		This polymer MW_n is >10,000; potential for irreversible lung damage as a result of lung overloading (Estimated)	Professional judgment; EPA, 2011	Based on SF polymer assessment guidance.
Skin Sensitization		**LOW: Estimated not to have potential for skin sensitization based on expert judgment. No data located.**		
	Skin Sensitization	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Estimated not to have potential for eye irritation based on expert judgment. No data located.**		
	Eye Irritation	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Dermal Irritation		**LOW: Estimated not to have potential for dermal irritation based on expert judgment. No data located.**		
	Dermal Irritation	Low potential for skin sensitization. (Expected)	Expert judgment	Estimated based on expert judgment.
Endocrine Activity		**This polymer is large, with a MW >1,000. It is not expected to have endocrine activity due to its poor bioavailability and inability to be readily metabolized in the body.**		
		Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
Immunotoxicity		**This polymer is large, with a MW >1,000. It is expected to have limited bioavailability and therefore has low potential for immunotoxicity.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment**;** EPA, 2010	Based on SF polymer assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		

TBBPA Glycidyl Ether, TBBPA Polymer CASRN 68928-70-1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Acute Toxicity	**LOW: Non-ionic polymers with a MW >1,000 and negligible water solubility are estimated to display no effects at saturation (NES). These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for those materials that display NES.**		
Fish LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid LC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity	**LOW: Non-ionic polymers with a MW >1,000 and negligible water solubility are estimated to display NES. These polymers display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed. Guidance for the assessment of aquatic toxicity hazard leads to a low potential for those materials that display NES.**		
Fish ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Daphnid ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
Green Algae ChV	NES	Professional judgment	The large MW, limited bioavailability and low water solubility suggest there will be NES.
ENVIRONMENTAL FATE			

TBBPA Glycidyl Ether, TBBPA Polymer CASRN 68928-70-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Transport		**The estimated negligible water solubility and estimated negligible vapor pressure indicate that this polymer is anticipated to partition predominantly to soil and sediment. The estimated Henry's Law Constant of $<10^{-8}$ atm-m^3/mole indicates that it is not expected to volatilize from water to the atmosphere. The estimated K_{oc} of >30,000 indicates that it is not anticipated to migrate from soil into groundwater and also has the potential to adsorb to sediment.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to have low vapor pressure and are not expected to undergo volatilization according to polymer assessment guidance.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	Professional judgment; EPA, 2010	Cutoff value used for large, high MW polymers. High MW polymers are expected to adsorb strongly to soil and sediment according to SF polymer assessment guidance.
	Level III Fugacity Model			No data located.
Persistence		**VERY HIGH: This polymer is large, with a MW >1,000. It is expected to have negligible water solubility and poor bioavailability to microorganisms indicating that neither biodegradation nor hydrolysis are expected to be important removal processes in the environment. Although debromination by photodegradation of polybrominated benzenes has been observed, this process is not anticipated to lead to ultimate removal of the material. As a result, a half-life for this high MW polymer of >180 days leads to a potential for very high persistence.**		
Water	**Aerobic Biodegradation**	Recalcitrant (Estimated)	Professional judgment; EPA, 2010	High MW polymers are expected to be non-biodegradable according to SF polymer assessment guidance.
	Volatilization Half-life for Model River	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	Professional judgment	Based on the magnitude of the estimated Henry's Law Constant.
Soil	**Aerobic Biodegradation**			No data located.

TBBPA Glycidyl Ether, TBBPA Polymer CASRN 68928-70-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Anaerobic Biodegradation			No data located.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**			No data located.
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Professional judgment	Bromine substituents may be susceptible to photolysis in the environment; however, this is expected to be a relatively slow process for a high MW brominated epoxy polymer and is not anticipated to result in the ultimate degradation of this substance.
	Hydrolysis	>1 year (Estimated)	Professional judgment	Given the limited solubility estimated for this material, hydrolysis is not anticipated to occur to an appreciable extent.
Environmental Half-Life		>180 days (Estimated)	Professional judgment	The substance is a high MW polymer and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to undergo removal by other degradative processes under environmental conditions.
Bioaccumulation		**LOW: Due to the large size and limited bioavailability of the high MW brominated epoxy polymer, it is of low potential for bioconcentration or bioaccumulation.**		

TBBPA Glycidyl Ether, TBBPA Polymer CASRN 68928-70-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Fish BCF	<100 (Estimated)	Professional judgment; EPA, 2010	Cutoff value for large, high MW, insoluble polymers according to SF polymer assessment guidance.
	BAF			No data located.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

CDC (Centers for Disease Control and Prevention). *Fourth national report on human exposure to environmental chemicals, updated tables*. Department of Health and Human Services. **2011.** http://www.cdc.gov/exposurereport/pdf/Updated_Tables.pdf (accessed on May 10, 2011).

[Polymer Assessment Guidance] EPA (Environmental Protection Agency). Sustainable Futures Summary Assessment. *Interpretive Assistance Document for Assessment of Polymers.* U.S. Environmental Protection Agency: Washington D.C. **2010**. http://www.epa.gov/oppt/sf/pubs/iad_polymers_042010.pdf as of September 2, 2011.

ESIS (European chemical Substances Information System) Classification, labeling and packaging of dangerous substances annex VI to regulation (EC) No 1272/2008 [Online]. http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=cla (accessed on May 10, **2011**).

ICL Industrial Products. *F-2300H.* Brominated Epoxy Polymer MSDS. http://www.icl-ip.com/brome/brome.nsf/viewAllByUNID/6A59162E67EFC8E2C225702900511DB6/$file/9223_enF-2300H.pdf (accessed on July 1, **2011**).

NICNAS (National Industrial Chemicals Notification and Assessment Scheme). Polybrominated flame retardants (PBFRs). Priority Existing Chemical Assessment Report No. 20. National Industrial Chemicals Notification and Assessment Scheme, June **2001.**

Triphenyl Phosphate

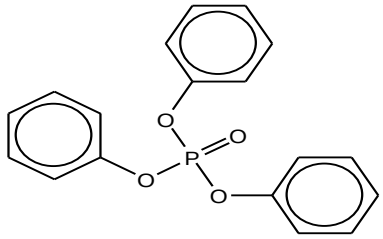
Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Triphenyl Phosphate	115-86-6	L	*M*	L	L	L	L	M	L		L	VL	VH	VH	L	M

Triphenyl Phosphate



CASRN: 115-86-6

MW: 326.29

MF: $C_{18}H_{15}O_4P$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: O=P(Oc1ccccc1)(Oc1ccccc1)Oc1ccccc1

Synonyms: Phosphoric acid, triphenyl ester (TSCA Inventory); TPP

Chemical Considerations: This is a discrete organic chemical with a MW below 1000. EPI v 4.0 was used to estimate physical/chemical and environmental fate values due to an absence of experimental data. Measured values from experimental studies were incorporated into the estimations.

Polymeric: No
Oligomers: Not applicable

Metabolites, Degradates and Transformation Products: Diphenyl phosphate

Analog: No analog
Endpoint(s) using analog values: Not applicable

Analog Structure: Not applicable

Structural Alerts: None

Risk Phrases:
R50/53: Very toxic to aquatic organisms. May cause long-term adverse effects in the aquatic environment (OECD SIDS, 2002).

Hazard and Risk Assessments: DfE Alternatives Assessment for Furniture Flame Retardancy Partnership, September, 2005 (U.S. EPA, 2005)

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory and is subject to a Section 4 test rule.

Triphenyl Phosphate CASRN 115-86-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	50.5 (Measured)	Lide, 2008	Adequate.
Boiling Point (°C)	245 at 11 mmHg (Measured)	O'Neil, 2006	Adequate.
	>300 (Estimated)	EPI; EPA, 1999	Cutoff value for high boiling point compounds according to HPV assessment guidance.
Vapor Pressure (mm Hg)	$6.28x10^{-6}$ (Extrapolated)	Dobry and Keller, 1957	Adequate.
Water Solubility (mg/L)	1.9 (Measured)	Saeger et al., 1979	Adequate.
Log K_{ow}	4.59 (Measured)	Hansch and Leo, 1995	Adequate.
Flammability (Flash Point)	220°C (Measured)	Lewis, 2001	Adequate.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
pK_a	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Triphenyl phosphate is hydrolyzed in the liver to produce diphenyl phosphate as the primary metabolite.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	Triphenyl phosphate is hydrolyzed in rat liver homogenate to produce the metabolite diphenyl phosphate (Measured)	OECD SIDS, 2002	Reported in a secondary source.
Acute Toxicity		**LOW: Oral LD_{50} in rats and mice is >5,000 mg/kg and the dermal LD_{50} in rabbits is >7,900 mg/kg. No adequate data were located to assess the toxicity of inhalation exposure.**		
Acute Lethality	**Oral**	Rat, mouse, oral LD_{50} >5,000 mg/kg (Measured)	OECD SIDS, 2002	Reported in a secondary source.
		Several rat, oral, LD_{50} >6,400 mg/kg (Measured)	ATSDR, 2009	Reported in a secondary source.
	Dermal	Rabbit dermal LD_{50} >10,000 mg/kg (Measured)	OECD SIDS, 2002	Reported in a secondary source.
		Rabbit dermal LD_{50} >7,900 mg/kg (Measured)	ATSDR, 2009	Reported in a secondary source.
	Inhalation	Rat LC_{50} >200,000 mg/m^3 (dust), 1-hour exposure, 14-day observation (Measured)	ATSDR, 2009	Reported in a secondary source. Insufficient exposure time (1 hour), no data on method or GLP.
Carcinogenicity		**MODERATE: OncoLogic modeling indicates a marginal to low potential for carcinogenicity. No long-term carcinogenicity assays were found.**		
	OncoLogic Results	Marginal (Estimated)	OncoLogic, 2008	
	Carcinogenicity (Rat and Mouse)	Mouse lung adenoma test: Male A/St mice (20/group) received i.p. injections of either 20 mg/kg (18/6 weeks); 40 mg/kg (3/1 week); or 80 mg/kg. No significant increase in incidence of adenoma compared to negative controls, and positive control (urethane) produced 19.6 tumors/mouse with 100% survival. (Measured)	OECD SIDS, 2002	Reported in a secondary source. Nonstandard study, limited histopathology and short-duration, reported in a secondary source.

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Combined Chronic Toxicity/ Carcinogenicity			No data located.
Genotoxicity		**LOW: Triphenyl phosphate was not mutagenic in bacteria or mammalian cells *in vitro* and did not cause chromosomal aberrations in vitro. In addition, triphenyl phosphate did not result in DNA damage in hamster fibroblast cells.**		
	Gene Mutation *in vitro*	Negative, Ames assay in *Salmonella typhimurium* strains TA98, TA100, TA1537, TA1538 with and without metabolic activation	ATSDR, 2009, ECHA, 2012	Reported in a secondary source.
		Negative, forward mutation assay in mouse lymphoma L5178Y cells (Measured)	OECD SIDS, 2002, ECHA, 2012	Reported in a secondary source.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	Negative in chromosome aberration test in Chinese hamster V79 cells; with and without metabolic activation.	ECHA, 2012	Reported in a secondary source.
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair	Negative, unscheduled DNA synthesis in hamster fibroblast cells (Measured)	OECD SIDS, 2002	Reported in a secondary source.
	Other (Mitotic Gene Conversion)	Negative, mitotic gene conversion assay in *Saccharomyces cerevisiae* with and without activation (Measured)	OECD SIDS, 2002	Reported in a secondary source.
Reproductive Effects		**LOW: Based on a rat oral reproductive/developmental NOAEL = 690 mg/kg-bw/day for reproductive effects (highest dose tested). In addition, no histopathological effects on reproductive organs were reported following 3 weeks of dermal exposure in rabbits.**		
	Reproduction/ Developmental Toxicity Screen			No data located.

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen	Reproductive/developmental dietary study (91 days premating and continuing through gestation), 40 male and 40 female rats/group, test compound concentrations of 0, 0.25, 0.50, 0.75, or 1.0% (~0, 166, 341, 516 or 690 mg/kg-bw/day, respectively). No signs of parental toxicity, no reproductive effects (number pregnant, corpora lutea, implantations, implantation efficiency, resorptions). NOAEL (reproductive effects) = 690 mg/kg-bw/day (highest dose tested) (Measured) LOAEL = not identified; there were no effects at the highest dose tested.	OECD SIDS, 2002; ATSDR, 2009	Reported in a secondary source.
	Reproduction and Fertility Effects	Rabbits, dermal (clipped, intact), 5x/week, 3 weeks, 50% solution in ethanol; no effect on the reproductive organs reported up to the highest dose tested (1,000 mg/kg/day) NOAEL = 1,000 mg/kg/day (Measured)	OECD SIDS, 2002	Reported in a secondary source. Organs examined by histopathology; there were no effects at the highest dose tested; dermal repeated-dose study.

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**LOW: Based on a rat oral reproductive/developmental NOAEL = 690 mg/kg-bw/day for fetal effects (highest dose tested).**		
	Reproduction/ Developmental Toxicity Screen	Reproductive/ developmental (dietary) study, 91 days premating (males and females), continuing through gestation and lactation (females only), 40 male and 40 female rats/group, test compound concentrations of 0, 0.25, 0.50, 0.75, or 1.0% (~0, 166, 341, 516 or 690 mg/kg-bw/day, respectively), no effects on fetal endpoints (viability, early or late deaths, fetal weight, length or distribution) or skeletal anomalies. NOAEL (developmental effects) = 690 mg/kg-bw/day (Measured)	OECD SIDS, 2002; ATSDR, 2009	Reported in a secondary source. A LOAEL was not identified; there were no effects at the highest dose tested.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Prenatal Development			No data located.
	Postnatal Development			No data located.
Neurotoxicity		**LOW: Based on an adult rat neurotoxicity screening battery NOAEL = 711 mg/kg-bw/day; all other experimental results are consistent with this hazard designation.**		
	Acute and 28-day Delayed Neurotoxicity of Organophosphorus Substances (Hen)	Two female hens/dose in delayed neurotoxicity test, gavage, 2,000, 3,000, 5,000, 8,000, or 12,500 mg/kg, no signs of toxicity in-life or at necropsy NOAEL ≥12,500 mg/kg (Measured)	OECD SIDS, 2002	Reported in a secondary source. No data on test substance purity.

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Several acute oral studies in hens, administered doses up to 12,500 mg/kg, generally found no signs of paralysis, histopathological changes in examined nerve tissues, or behavior immediately after or during observation periods of up to 36 days. However, blood cholinesterase was decreased by up to 87% in studies where it was measured. NOAEL = >12,500 mg/kg (Measured)	OECD SIDS, 2002	Reported in a secondary source. No data on test substance purity.
	Neurotoxicity Screening Battery (Adult)	4-month dietary study, 10 rats/dose, 0.25, 0.5, 0.75 or 1% test concentration (161, 345, 517 or 711 mg/kg-bw/day, respectively), no neurobehavioral effects (open field, accelerating rotarod, forelimb grip strength and negative geotaxis examinations) NOAEL = 711 mg/kg-bw-day (highest dose tested) (Measured)	ATSDR, 2009	Reported in a secondary source.
Repeated Dose Effects		**MODERATE: Based on reduced body weight in rats administered triphenyl phosphate in the diet for 28-days. The LOAEL of 161.4 mg/kg-day falls within the Moderate hazard designation range (DfE criteria are for 90-day repeated dose studies; criteria values are tripled for chemicals evaluated in 28-day studies making the moderate hazard range between 30 and 300 mg/kg-day).**		

Triphenyl Phosphate CASRN 115-86-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	35-day repeated-dose oral (dietary) study, 5 male rats/group, test compound concentrations of 0, 0.5, and 5.0% (~0, 350, and 3,500 mg/kg-day, respectively), with a 0.1% (~70 mg/kg-day) dose replacing the high dose group after 3 days. Slight reduction in body weight gain and increase in liver weight in 350 mg/kg-day dose group. NOAEL = 70 mg/kg-day LOAEL = 350 mg/kg-day (Measured)	OECD SIDS, 2002	Reported in a secondary source. Limited study details provided.
	4-month repeated-dose dietary study, Sprague-Dawley rats, 10 rats/dose, 0.25, 0.5, 0.75 or 1% test concentration (161, 345, 517 or 711 mg/kg-bw/day, respectively), reduced body weight gain (11%) at 345 mg/kg-bw/day. NOAEL = 161 mg/kg-bw/day LOAEL = 345 mg/kg-bw/day (Measured)	ATSDR, 2009	Reported in a secondary source.

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		21-day repeated-dose dermal study, 10 male and 10 female rabbits/group, test compound concentrations of 0, 100, and 1,000 mg/kg-bw/day, no mortality, clinical symptoms, or changes in body weight, hematology, clinical chemistry, necropsy, organ weights and histopathology reported; only decreased acetyl cholinesterase levels in plasma, erythrocytes and brain were reported and not considered to be of toxicological relevance as there was no clinical or histological correlation. NOAEL = 1,000 mg/kg-bw/day (Measured)	OECD SIDS, 2002	Reported in a secondary source. Treatment period only 21 days.
		28-day repeated dose oral exposure study in rats. 0, 250, 1000, 4000 ppm in diet. Effects on body weights were observed Male: NOAEL = 250 ppm (23.5 mg/kg-day) LOAEL = 1000 ppm (161.4 mg/kg-day)	ECHA, 2012	Reported in secondary source. DfE criteria are for 90-day repeated dose studies. Criteria values are tripled for chemicals evaluated in 28-day studies.
Skin Sensitization		**LOW: Based on an experimental study in guinea pigs indicating that triphenyl phosphate is not a skin sensitizer.**		
	Skin Sensitization	Several human case studies have reported allergic dermatitis; 15 of 23,192 (0.065%) human volunteers patch tested from 1950 to 1962 had positive reactions to cellulose acetate film containing 7-10% triphenyl phosphate and 3-4% phthalic esters (Measured)	OECD SIDS, 2002	Reported in a secondary source. Limited study details provided; patch testes conducted with mixtures; unclear which component of mixture caused low incidence of sensitization.
		A confidential skin sensitization study with negative results in guinea pigs (Measured)	Confidential study	Reported in a confidential study.

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		None of the patients tested in two separate studies of 343 and 174 patients, respectively, had sensitization reactions to triphenyl phosphate	OECD SIDS, 2002	Reported in a secondary source. Limited study details provided.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Triphenyl phosphate is mildly irritating to the eyes with clearing within 72 hours.**		
	Eye Irritation	Mild irritation in rabbit eyes, clearing within 72 hours	OECD SIDS, 2002	Reported in a secondary source.
Dermal Irritation		**VERY LOW: Triphenyl Phosphate is not a skin irritant based on one study in rabbits.**		
	Dermal Irritation	Non-irritant, rabbit (Measured)	ATSDR, 2009	Reported in a secondary source.
Endocrine Activity		**Triphenyl phosphate was found to be inactive in an estrogen-receptor binding assay; however, it was shown to be a moderate androgen-receptor (AR) binder in a competitive binding assay. Triphenyl phosphate was also shown to inhibit human AR in the absence of agonist and to inhibit testosterone-induced AR activity.**		
		Inactive in a binding assay with the rat uteri estrogen receptor from ovariectomized Sprague-Dawley rats (Measured)	ATSDR, 2009	Reported in a secondary source.
		Moderate binding in a competitive androgen-receptor (AR) binding assay using recombinant rat protein expressed in *Escherichia coli*. (Measured)	ATSDR, 2009	Reported in a secondary source.
		Inhibited AR activity in COS-1 cells transfected with human AR both in the absence of agonist, as well as inhibited testosterone-induced AR activity by 30-40%. (Measured)	ATSDR, 2009	Reported in a secondary source.

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Immunotoxicity		**Oral exposure of rats to triphenyl phosphate for 4 months and dermal exposure of rabbits for 3 weeks produced no effects on immune function parameters.**		
	Immune System Effects	120-day dietary study, rats, 0, 0.25, 0.5, 0.75, and 1% of triphenyl phosphate (~0, 161, 345, 517 and 711 mg/kg-bw/day); initial, secondary, and tertiary immunizations with sheep red blood cells performed at 60, 81, and 102 days, respectively. No significant effects were reported on the weight and histopathology of the spleen, thymus and lymph nodes, and no significant changes to the humoral response were reported. NOEL = 711 mg/kg/day (Measured)	ATSDR, 2009	Reported in a secondary source.
		Rabbits, up to 1,000 mg/kg-bw/day, applied 5 days/week for 3 weeks to intact or abraded skin had no gross or microscopic effects on the spleen, thymus, or lymph nodes. (Measured)	ATSDR, 2009	Reported in a secondary source.
ECOTOXICITY				
ECOSAR Class		Esters (phosphate), Esters		
Acute Toxicity		**VERY HIGH: Based on experimental fish 96-hour LC_{50} values of 0.4 and 0.85 mg/L.**		
Fish LC_{50}		Fish 96-hour LC_{50} = 0.4 mg/L (Experimental)	OECD SIDS, 2002	Reported in a secondary source.
		Fish 96-hour LC_{50} = 0.85 mg/L (Experimental)	OECD SIDS, 2002	Reported in a secondary source. Guideline study.
		Fish 96-hour LC_{50} = 1.47 mg/L (Estimated) ECOSAR: Esters	EPI	
		Fish 96-hour LC_{50} = 1.24 mg/L (Estimated) ECOSAR: Esters (phosphate)	EPI	

Triphenyl Phosphate CASRN 115-86-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Fish 96-hour LC_{50} = 1.62 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
Daphnid LC_{50}	Daphnid 48-hour LC_{50} = 1.28 mg/L (Experimental)	FMC Industrial Chemical Division, 1979	Sufficient study details reported.
	Daphnid 48-hour LC_{50} = 2.16 mg/L (Estimated) ECOSAR: Esters	EPI	No Effects at Saturation (NES): The LC_{50} value exceeds the water solubility (1.9 mg/L); NES are predicted for these endpoints.
	Daphnid 48-hour LC_{50} = 1.98 mg/L (Estimated) ECOSAR: Esters (phosphate)	EPI	NES: The LC_{50} value exceeds the water solubility (1.9 mg/L); NES are predicted for these endpoints.
	Daphnid 48-hour LC_{50} = 1.28 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Daphnid 48-hour LC_{50} = 1,000 µg/L (Experimental)	Mayer et al., 1981	Sufficient study details reported.
Other Freshwater Invertebrate LC_{50}	*Mysidopsis bahia* 96-hour LC_{50} > 0.18 - 0.32 mg/L (Experimental)	OECD SIDS, 2002	Reported in a secondary source.
Green Algae EC_{50})	Green algae 96-h EC_{50} = 2.0 mg/L (Experimental)	OECD SIDS, 2002	Reported in a secondary source.
	Green algae 96-h EC_{50} = 2.0 mg/L (Experimental)	Mayer et al., 1981	Sufficient study details reported
	Green algae 96-hour EC_{50} = 0.70 mg/L (Estimated) ECOSAR: Esters	EPI	
	Green algae 96-hour EC_{50} = 2.71 mg/L (Estimated) ECOSAR: Esters (phosphate)	EPI	NES: The LC_{50} value exceeds the water solubility (1.9 mg/L); NES are predicted for these endpoints.
	Green algae 96-hour EC_{50} = 1.59 mg/L (Estimated) ECOSAR: Neutral organics	EPI	

Triphenyl Phosphate CASRN 115-86-6			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Chronic Aquatic Toxicity	**VERY HIGH: Based on an experimental fish 30-day LOEC = 0.037 mg/L.**		
Fish ChV	Fish 30-day LOEC = 0.23 mg/L (Experimental)	OECD SIDS, 2002	Reported in a secondary source. Guideline study.
	Oncorhynchus mykiss 30-day LOEC = 0.037 mg/L (Experimental)	ECHA, 2012	Reported in a secondary source.
	Fish 32/33-day ChV = 0.071 mg/L (Estimated) ECOSAR: Esters	EPI	
	Fish ChV = 0.10 mg/L (Estimated) ECOSAR: Esters (phosphate)	EPI	
	Fish ChV = 0.15 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
Daphnid ChV	Daphnid ChV = 0.186 mg/L (Estimated) ECOSAR: Neutral organic	EPI	
	Daphnid 21-day ChV = 0.699 mg/L (Estimated) ECOSAR: Esters	EPI	
	Daphnid ChV = 0. 381 mg/L (Estimated) ECOSAR: Esters (phosphate)	EPI	
Green Algae ChV	Green algae ChV = 0.925 mg/L (Estimated) ECOSAR: Neutral organics	EPI	
	Green algae ChV = 0.408 mg/L (Estimated) ECOSAR: Esters	EPI	
	Green algae ChV = 948.129 mg/L (Estimated) ECOSAR: Esters (phosphate)	EPI	NES: The LC_{50} value exceeds the water solubility (1.9 mg/L); NES are predicted for these endpoints.

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**Based on the Level III fugacity models incorporating the located property data, triphenyl phosphate is expected to partition primarily to soil. Triphenyl phosphate is expected to have moderate mobility in soil, based on measured K_{oc} values in silty clay, loamy sand and silt loam. Leaching through soil to groundwater may occur, though it is not expected to be an important transport mechanism. Estimated volatilization half-lives indicate that it will be non-volatile from surface water. Volatilization from dry surface is also not expected based on its vapor pressure. In the atmosphere, triphenyl phosphate is expected to exist in both the vapor phase and particulate phase, based on its vapor pressure. Particulates may be removed from air by wet or dry deposition.**		
	Henry's Law Constant (atm-m^3/mole)	$1.2x10^{-5}$ (Measured)	Mayer et al., 1981; Huckins et al., 1991	Adequate.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	2,514–3,561 in silty clay, loamy sand and silt loam (Measured)	Anderson et al., 1993	Adequate.
	Level III Fugacity Model	Air = <1% (Estimated) Water = 15% Soil = 75% Sediment = 9.6%	EPI	

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Persistence		**LOW: The persistence of triphenyl phosphate is based on experimental data. Under aerobic conditions in a Japanese MITI ready biodegradability test (OECD Test Guidelines (TG) 301C), 90% biodegradation of triphenyl phosphate occurred after 28 days, and 93.8% triphenyl phosphate removal as dissolved organic carbon (DOC) occurred over 20 days in an OECD 303A guideline study. TPP does not meet the criteria for very low persistence because the ready test values do not occur within a 10-day window. In loamy sand, a half-life of 37 days was observed under aerobic conditions. Triphenyl phosphate was determined to be inherently biodegradable in a river die-away test, after degrading 100% over 3 days in river water. Triphenyl phosphate may degrade under anaerobic conditions, with primary degradation of 31.1% after 3 days (89.7% after 40 days) in river sediment. However, it is not expected to significantly partition to sediment, and removal under anaerobic conditions is not anticipated to be an important fate process. Triphenyl phosphate will undergo hydrolysis under alkaline conditions, with half-lives of 3 days at pH 9; it is relatively stable to hydrolysis under neutral and acidic conditions, with half-lives of 28 days at pH 5 and 19 days at pH 7. Triphenyl phosphate is not expected to be susceptible to direct photolysis by sunlight, since it does not absorb light at wavelengths >290 nm. The atmospheric half-live of vapor-phase triphenyl phosphate is estimated to be 12 hours.**		
Water	**Aerobic Biodegradation**	Inherently Biodegradable: Degraded 100% after 3 days in river water (River die-away test) (Measured)	OECD SIDS, 2002	Adequate, guideline study.
	Volatilization Half-life for Model River	13 days (Estimated)	EPI	
	Volatilization Half-life for Model Lake	150 days (Estimated)	EPI	
Soil	**Aerobic Biodegradation**	Ready Test: MITI-I (OECD TG 301C). 90% biodegradation detected after 28 days at 100 ppm in 30 ppm activated sludge (Measured)	MITI, 1998	Adequate, guideline study.
		93.8% removal as DOC over 20 days (OECD 303A), using initial concentration of 5 mg/L with activated sludge. (Measured)	OECD SIDS, 2002	Adequate, guideline study.

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Anaerobic Biodegradation	Primary degradation: 31.1% removal after 3 days in river sediment; 89.7% removal after 40 days (Measured)	OECD SIDS, 2002	Adequate, guideline study.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation	Primary degradation: 43.3% removal after 3 days in river sediment; 86.9% removal after 40 days (Measured)	OECD SIDS, 2002	Adequate, guideline study.
Air	**Atmospheric Half-life**	12 hours (Estimated)	EPI	
Reactivity	**Photolysis**	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	Triphenyl phosphate does not contain functional groups that would be expected to absorb light of wavelengths >290 nm.
	Hydrolysis	Half-lives at 25°C: >28 days at pH 5; 19 days at pH 7; 3 days at pH 9 (Measured)	OECD SIDS, 2002	Adequate, guideline study.
Environmental Half-Life		In loamy sand, observed half-lives of 37 days (aerobic) and 21 days (anaerobic) (Measured)	OECD SIDS, 2002	Adequate, guideline study.
		75 days (Estimated)	EPI, PBT Profiler	Half-life estimated for the predominant compartment, as determined by EPI and the PBT Profiler methodology.
Bioaccumulation		**MODERATE: There is moderate concern for bioaccumulation based on experimental BCF values.**		
	Fish BCF	132–364 (Rainbow trout) (Measured)	Mayer et al., 1981	Adequate.
		271(Rainbow trout) (Measured)	Monsanto Chemical Co, 1982	
	BAF	73 (Estimated)	EPI	

Triphenyl Phosphate CASRN 115-86-6				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		Several studies on environmental monitoring have appeared; triphenyl phosphate has been detected in drinking water, surface water, sediment, and in ambient air (OECD SIDS, 2002).		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		Detected in human adipose tissue (NHATS, 1989). This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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Tris(tribromoneopentyl) Phosphate

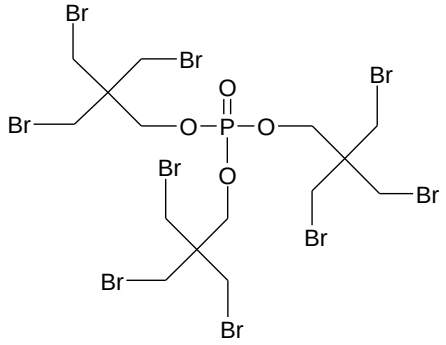
Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Tris(tribromoneopentyl) Phosphate	19186-97-1	*L*	*M*	*M*	*L*	*H*	*H*	*M*	*H*		*L*	*L*	*L*	*L*	*H*	*M*

Tris(tribromoneopentyl) Phosphate



CASRN: 19186-97-1

Molecular Weight (MW): 1,018.5

Molecular Formula: $C_{15}H_{24}Br_9O_4P$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: C(C(CBr)(CBr)CBr)OP(=O)(OCC(CBr)(CBr)CBr)OCC(CBr)(CBr)CBr

Synonyms: 1-Propanol, 3-bromo-2,2-bis(bromomethyl)-, 1,1',1"-phosphate (TSCA Inventory); 1-Propanol, 3-bromo-2,2-bis(bromomethyl)-, phosphate (3:1); 3-Bromo-2,2-bis(bromomethyl)propan-1-ol, phosphate (3:1); Tris[3-bromo-2,2-bis(bromomethyl)propyl]phosphate; Tris(tribromoneopentyl) phosphate; Tris[2,2-bis(bromomethyl)-3-bromopropyl] phosphate; Tris[3-bromo-2,2-bis(bromomethyl)propyl] phosphate; CR-900; Flame Cut 175; Flame Cut 175R; TPB 3070; FR 370; FR 372; Kronitex PB 370; Reoflam FR 370

Chemical Considerations: This is a discrete organic chemical with a MW slightly greater than 1000. EPI v 4.0 was used to estimate physical/chemical and environmental fate values due to an absence of experimental data. To provide robust estimates, physical-chemical property data from experimental studies were incorporated into the estimation software.

Polymeric: No
Oligomers: Not applicable

Metabolites, Degradates and Transformation Products: None

Analog: No analog
Endpoint(s) using analog values: Not applicable

Analog Structure: Not applicable

Structural Alerts: None

Risk Phrases: Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).

Hazard and Risk Assessments: None identified

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	183 (Measured)	Fisk et al., 2003	Adequate. Consistent values, which span a relatively narrow range, have been reported in secondary sources.
	182-184 (Measured)	NICNAS, 2001	
	180-182 (Measured)	Harju et al., 2009	
Boiling Point (°C)	>300 (Estimated)	EPI; EPA, 1999	Cutoff value for high boiling compounds according to HPV assessment guidance.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	EPI; EPA, 2011	Cutoff value for nonvolatile compounds according to SF assessment guidance.
Water Solubility (mg/L)	0.9 (Measured)	NICNAS, 2001; Fisk et al., 2003	Adequate.
Log K_{ow}	8.1 (Estimated)	EPI	This compound may lie just outside of the MW domain for the estimation method, although the results are consistent with a high MW material with limited water solubility.
	3.7 (Measured)	NICNAS, 2001; Fisk et al., 2003	Value inconsistent with measured water solubility. Reported in a secondary source; study details and test conditions were not provided.
Flammability (Flash Point)	388.8°C (Measured)	ChemNet, 2011	Adequate.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH	Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
pK_a		Not applicable	Professional judgment	Does not contain functional groups that are expected to ionize under environmental conditions.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Tris(tribromoneopentyl) phosphate, as a neat material, is estimated to not be absorbed through the skin and have poor skin absorption when in solution. Tris(tribromoneopentyl) phosphate is expected to have poor absorption via the lungs and gastrointestinal (GI) tract. This material is a potential alkylating and crosslinking agent.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	Not absorbed through the skin as a neat material and poor absorption through skin when in solution; poor absorption through the lung and GI tract (Estimated by analogy)	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/chemical properties.
Acute Mammalian Toxicity		**LOW: Estimated to have low potential for acute toxicity based on expert judgment.**		
Acute Lethality	**Oral**	Low potential for acute toxicity (Estimated)	Expert judgment	Estimated based on expert judgment.
	Dermal			
	Inhalation			
Carcinogenicity		**MODERATE: Estimated to have moderate potential for carcinogenicity based on a mechanistic consideration of the potential for alkylation and crosslinking using professional judgment.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)	There is potential for carcinogenicity based on a consideration of the mechanistic potential for alkylation and crosslinking. (Estimated by analogy)	Professional judgment	Estimated based on professional judgment.
	Combined Chronic Toxicity/ Carcinogenicity			

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Genotoxicity		**MODERATE: Estimated to have moderate potential for genotoxicity based on a mechanistic consideration of the potential for alkylation and crosslinking activity using professional judgment.**		
	Gene Mutation *in vitro*	There is potential for mutagenicity based on the potential for alkylation and crosslinking. (Estimated by analogy)	Professional judgment	Estimated based on professional judgment.
	Gene Mutation *in vivo*			
	Chromosomal Aberrations *in vitro*			
	Chromosomal Aberrations *in vivo*			
	DNA Damage and Repair			
	Other (Mitotic Gene Conversion)			
Reproductive Effects		**LOW: Estimated to have low potential for reproductive effects based on expert judgment.**		
	Reproduction/ Developmental Toxicity Screen	Low potential for acute toxicity (Estimated)	Expert judgment	Estimated based on expert judgment.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Reproduction and Fertility Effects			

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**HIGH: Estimated to have high potential for developmental effects based on a mechanistic consideration of the potential for alkylation and crosslinking using professional judgment.**		
	Reproduction/ Developmental Toxicity Screen **Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen** **Prenatal Development** **Postnatal Development**	There is potential for developmental effects based on a mechanistic consideration of the potential for alkylation and crosslinking. (Estimated by analogy)	Professional judgment	Estimated based on professional judgment.
Neurotoxicity		**HIGH: Estimated to have high potential for neurotoxicity based on the potential for the neopentyl alcohol groups acting as leaving groups, based on professional judgment.**		
	Neurotoxicity Screening Battery (Adult)	There is a potential for neurotoxicity using a mechanistic analysis based on the formation of neopentyl alcohol groups due to their ability to act as good leaving groups. (Estimated by analogy)	Professional judgment	Estimated based on professional judgment.
Repeated Dose Effects		**MODERATE: There is uncertain potential for liver effects based on the bromo substituents of tris(tribromoneopentyl) phosphate, based on professional judgment.**		
		There is an uncertain potential for liver effects based on a mechanistic consideration of the reactions of the bromo substituents of this chemical. (Estimated by analogy)	Professional judgment	Estimated based on professional judgment.

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Skin Sensitization		**HIGH: Estimated to have high potential for skin sensitization based on a mechanistic consideration of the potential for alkylation and crosslinking, based on professional judgment.**		
	Skin Sensitization	There is potential for skin sensitization based on a mechanistic consideration of the potential for alkylation and crosslinking. (Estimated by analogy)	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/chemical properties.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Estimated to have low potential for eye irritation based on expert judgment.**		
	Eye Irritation	Low potential for eye irritation. (Estimated)	Expert judgment	Estimated based on expert judgment.
Dermal Irritation		**LOW: Estimated to have low potential for dermal irritation based on expert judgment.**		
	Dermal Irritation	Low potential for skin irritation. (Estimated)	Expert judgment	Estimated based on expert judgment.
Endocrine Activity		**Estimated not to have potential for endocrine activity based on expert judgment.**		
		Low potential for endocrine activity. (Estimated)	Expert judgment	Estimated based on expert judgment.
Immunotoxicity		**Estimated to have low potential for immunotoxicity based on expert judgment.**		
	Immune System Effects	Low potential for immunotoxicity. (Estimated)	Expert judgment	Estimated based on expert judgment.
ECOTOXICITY				
ECOSAR Class		Esters; Esters (phosphate)		
Acute Toxicity		**LOW: Tris(tribromopentyl) phosphate's large MW, limited bioavailability and low water solubility suggest there will be no effects at saturation (NES). The estimated log K_{ow} of 8.1 also is indicative of NES based on ECOSAR cutoff values.**		
Fish LC_{50}		Fish 96-hour LC_{50} >10 mg/L (test concentration exceeded water solubility)	Fisk et al., 2003	Inadequate; details are missing as this is a review on various chemicals. In addition, the LC_{50} > the highest test concentration.

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Fish 96-hour LC_{50} = 0.007 mg/L ECOSAR: Esters (phosphate) (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0.
	Fish 96-hour LC_{50} = 0.006 mg/L ECOSAR: Neutral organics (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0.
Daphnid LC_{50}	Daphnia 48-hour LC_{50} =0.045 mg/L ECOSAR: Esters (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; The log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0.
	Daphnia 48-hour LC_{50} = 0.115 mg/L ECOSAR: Esters (phosphate) (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0.
	Daphnia 48-hour LC_{50} = 0.007 mg/L ECOSAR: Neutral organics (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0.

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Other Freshwater Invertebrate LC_{50}	Mysid shrimp 96-hour LC_{50} = 0.003 mg/L ECOSAR: Esters (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 5.0.
Green Algae EC_{50}	Green algae 96-hour EC_{50} = 0.010 mg/L ECOSAR: Esters (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4.
	Green algae 96-hour EC_{50} = 0.022 mg/L ECOSAR: Esters (phosphate) (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4.
	Green algae 96-hour EC_{50} = 0.037 mg/L ECOSAR: Neutral organics (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 6.4.
Chronic Aquatic Toxicity	**LOW: The large MW, limited bioavailability, and low water solubility suggest there will be NES. The estimated log K_{ow} of 8.1 is indicative of NES based on ECOSAR cutoff values.**		
Fish ChV	Fish 32/33 day ChV = 0.00101 mg/L ECOSAR: Esters (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0.

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
	Fish ChV = 0.000498 mg/L ECOSAR: Esters (phosphate) (Estimated)	EPI	NES: the large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0.
	Fish ChV = 0.000495 mg/L ECOSAR: Neutral organics (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0.
Daphnid ChV	Daphnid 21-day ChV = 0.006 mg/L ECOSAR: Esters (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0.
	DaphnidChV = 0.0019 mg/L ECOSAR: Esters (phosphate) (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0
	Daphnid ChV = 0.00192 mg/L ECOSAR: Neutral organics (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0.

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
Saltwater Invertebrate ChV	Mysid shrimp ChV = $6.8x10^{-7}$ mg/L ECOSAR: Esters (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0.
Green Algae ChV	Green algae ChV = 0.018 mg/L ECOSAR: Esters (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0.
	Green algae ChV = 0.036 mg/L ECOSAR: Esters (phosphate) (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0.
	Green algae ChV = 0.040 mg/L ECOSAR: Neutral organics (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0.
Earthworm Subchronic Toxicity	Earthworm 14-day EC_{50} = 148 830 mg/L ECOSAR: Esters (Estimated)	EPI	NES: The large MW, limited bioavailability and low water solubility suggest there will be NES; the log K_{ow} of 8.1 for this chemical exceeds the SAR limitation for log K_{ow} of 8.0.

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL FATE				
Transport		**Evaluation of tris(tribromoneopentyl) phosphate transport is based entirely on estimations from QSARs. Tris(tribromoneopentyl) phosphate is expected to have low mobility in soil based on its expected strong absorption to soil. If released to the atmosphere, tris(tribromoneopentyl) phosphate is likely to exist solely as particulate. As a particulate, atmospheric oxidation is not expected to be a significant route of environmental removal. Based on the Henry's Law constant, volatilization from water or moist soil is not expected to occur at an appreciable rate. Level III fugacity models indicate that tris(tribromoneopentyl) phosphate will partition predominantly to the soil.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	EPI; Professional judgment	Cutoff value for nonvolatile compounds.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	EPI; EPA, 2011	Cutoff value for nonmobile compounds according to SF assessment guidance.
	Level III Fugacity Model	Air = <1% (Estimated) Water = 1% Soil = 64% Sediment = 35%	EPI	
Persistence		**HIGH: This substance has a MW slightly >1,000. It is expected to have negligible water solubility and poor bioavailability to microorganisms indicating that biodegradation is not expected to be an important removal process in the environment. Estimated hydrolysis half-lives of approximately 10 years indicate that this will not be an important environmental removal process. Tris(tribromoneopentyl) phosphate does not contain functional groups that would be expected to absorb light at environmentally significant wavelengths. As a result, tris(tribromoneopentyl) phosphate is expected to have high potential for environmental persistence.**		
Water	**Aerobic Biodegradation**	Weeks-months (primary survey model); Recalcitrant (ultimate survey model)	EPI	Although this compound may lie just outside of the MW domain for the estimation method, the results are consistent with a high MW material that is not expected to be readily assimilated.
	Volatilization Half-life for Model River	>1 year (Estimated)	EPI	Based on the magnitude of the estimated Henry's Law Constant.

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Volatilization Half-life for Model Lake	>1 year (Estimated)	EPI	Based on the magnitude of the estimated Henry's Law Constant.
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation	Probable (Anaerobic-methanogenic biodegradation probability model)	EPI; Professional judgment	The model predictions are being driven by reduction of the bromine substituent. Under environmental conditions, the rate for anaerobic degradation will likely be attenuated due to the low water solubility and limited bioavailability of this material.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	Not a significant fate process (Estimated)	Professional judgment	This chemical is expected to exist in the particulate phase in the atmosphere.
Reactivity	**Photolysis**			No data located.
	Hydrolysis	pH 7 = 9.9 years (Estimated) pH 8 = 9.9 years	EPI	
	Pyrolysis			No data located.

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Environmental Half-life		>180 days (Estimated)	Professional judgment	The substance has a MW slightly >1,000 and is not anticipated to be assimilated by microorganisms. Therefore, biodegradation is not expected to be an important removal process. It is also not expected to be readily removed by other degradative processes under environmental conditions because of limited water solubility and lack of reactive functional groups.
Bioaccumulation		**MODERATE: The estimated BCF is >100 and <1,000.**		
	Fish BCF	609 (Estimated)	EPI	
	BAF	8.8 (Estimated)	EPI	
	Metabolism in Fish			No data located.

Tris(tribromoneopentyl) Phosphate CASRN 19186-97-1			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL MONITORING AND BIOMONITORING			
Environmental Monitoring	No data located.		
Ecological Biomonitoring	No data located.		
Human Biomonitoring	This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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NICNAS (National Industrial Chemicals Notification and Assessment Scheme). Polybrominated flame retardants (PBFRs) priority existing chemical assessment Report No. 20 National Occupational Health and Safety Commission, Australia. **2001**.

Tris(tribromophenoxy) Triazine

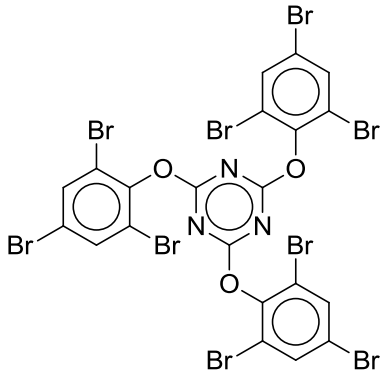
Screening Level Hazard Summary

This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

Chemical	CASRN	Human Health Effects											Aquatic Toxicity		Environmental Fate	
		Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Tris(tribromophenoxy) Triazine	25713-60-4	L	*L*	L	*L*	*L*	*L*	L	L		L	VL	*L*	*L*	VH	*H*

Tris(tribromophenoxy) Triazine



CASRN: 25713-60-4

MW: 1,067.43

MF: $C_{21}H_6Br_9N_3O_3$

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: c1(Br)c(Oc2nc(Oc3c(Br)cc(Br)cc3Br)nc(Oc3c(Br)cc(Br)cc3Br)n2)c(Br)cc(Br)c1

Synonyms: 1,3,5-Triazine, 2,4,6-tris(2,4,6-tribromophenoxy)- (TSCA Inventory); Tris(tribromophenoxy) triazine; FR 245; Tris(2,4,6-tribromophenoxy)-s-triazine; Tris(tribromophenoxy)-s-triazine; Tris(tribromophenyl) cyanurate

Chemical Considerations: This is a discrete organic chemical with a MW slightly greater than 1,000. EPI v 4.0 was used to estimate physical/chemical and environmental fate values due to an absence of experimental data.

Polymeric: No
Oligomers: Not applicable

Metabolites, Degradates and Transformation Products: Tribromophenol (NICNAS, 2006)

Analog: No analog
Endpoint(s) using analog values: Not applicable

Analog Structure: Not applicable

Structural Alerts: Reproductive toxicity, triazines (U.S. EPA, 2011a)

Risk Phrases: Not classified by Annex I Directive 67/548/EEC & IUCLID (Pakalin et al., 2007).

Hazard and Risk Assessments: None identified

U.S. EPA TSCA Regulatory Status: This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.

Tris(tribromophenoxy) Triazine CASRN 25713-60-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	228-229 (Measured) EC Directive 92/69/EEC A.1	NICNAS, 2006	Adequate; reported in a secondary source. Melting started at 216-218ºC, likely due to impurities in test substance.
Boiling Point (°C)	Decomposition at >275 (Measured) EC Directive 92/69/EEC A.1 using 99.5% pure test substance	NICNAS, 2006	Adequate; reported in a secondary source.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	EPI; EPA, 2011b	Cutoff value for nonvolatile compounds according to SF assessment guidance.
Water Solubility (mg/L)	$<10^{-3}$ at 20°C (Measured) OECD TG 105, GLP compliant	NICNAS, 2006	Adequate; reported in a secondary source. Reported value also corresponds to the cutoff value for nonsoluble compounds according to HPV assessment guidance.
Log K_{ow}	>10 (Estimated)	EPI; EPA, 2011b	Although this material may be outside the MW domain for the estimation model, the resulting value is consistent with that anticipated for a highly brominated, high MW substance. Cutoff value used according to SF assessment guidance.
Flammability (Flash Point)	Non flammable (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Explosivity	Not expected to form explosive mixtures with air (Estimated)	Professional judgment	No experimental data located; based on its use as a flame retardant.
Pyrolysis			No data located.
pH			No data located.

Tris(tribromophenoxy) Triazine CASRN 25713-60-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
pK_a				No data located; the high MW precludes the use of available estimation methods.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Tris(tribromophenoxy) triazine has a MW >1,000 and limited water solubility. There is no absorption expected for any route of exposure for this compound and is not expected to be absorbed, distributed or metabolized in the body. The lack of absorption is expected to result in low hazard potential.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No absorption expected for any route of exposure (Estimated)	Professional judgment	Estimated based on professional judgment.
Acute Mammalian Toxicity		**LOW: Tris(tribromophenoxy) triazine has a MW >1,000 and limited water solubility. It is expected to have limited bioavailability and therefore has low potential for acute mammalian toxicity. In addition, oral and dermal LD_{50} values >2,000 indicate a low level of toxicity.**		
Acute Lethality		Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2011	Based on SF discrete organic chemicals assessment guidance.
	Oral	Rat oral LD_{50} >2,000 mg/kg	NICNAS, 2006	Reported in a secondary source.
	Dermal	Rat dermal LD_{50} >2,000 mg/kg	NICNAS, 2006	Reported in a secondary source.
	Inhalation			No data located.
Carcinogenicity		**LOW: Tris(tribromophenoxy) triazine is expected to have limited bioavailability. It is estimated to have low potential for carcinogenicity based on professional judgment.**		
	OncoLogic Results	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2011	Based on SF discrete organic chemicals assessment guidance.
	Carcinogenicity (Rat and Mouse)			
	Combined Chronic Toxicity/ Carcinogenicity			
Genotoxicity		**LOW: Tris(tribromophenoxy) triazine was not mutagenic in *Salmonella typhimurium* and did not induce chromosome aberrations in human peripheral lymphocytes and L5178Y mouse lymphoma cells. Tris(tribromophenoxy) triazine is expected to have limited bioavailability and therefore has low potential for genotoxicity.**		

Tris(tribromophenoxy) Triazine CASRN 25713-60-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Gene Mutation *in vitro*	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2011	Based on SF discrete organic chemicals assessment guidance.
		Negative, Ames assay in *Salmonella typhimurium* strains TA1535, TA1537, TA98, TA100, with and without activation.	NICNAS, 2006	Reported in a secondary source.
	Gene Mutation *in vivo*			No data located.
	Chromosomal Aberrations *in vitro*	Negative, Mammalian Chromosome Aberration Test in cultured human peripheral lymphocytes, with and without activation. Precipitation was noted at the highest concentration tested.	NICNAS, 2006	Reported in a secondary source.
		Negative, Mammalian Cell Gene Mutation Test in L5178Y mouse lymphoma cells with and without activation. Precipitation was noted at the highest concentration tested.	NICNAS, 2006	Reported in a secondary source.
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair			No data located.
	Other (Mitotic Gene Conversion)			No data located.
Reproductive Effects		**LOW: Tris(tribromophenoxy) triazine is expected to have limited bioavailability. It is estimated to have low potential for reproductive effects based on professional judgment.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2011	Based on SF discrete organic chemicals assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			

Tris(tribromophenoxy) Triazine CASRN 25713-60-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Reproduction and Fertility Effects			
Developmental Effects		**LOW: Tris(tribromophenoxy) triazine is expected to have limited bioavailability. It is estimated to have low potential for developmental effects based on professional judgment.**		
	Reproduction/ Developmental Toxicity Screen	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2011	Based on SF discrete organic chemicals assessment guidance.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			
	Prenatal Development			
	Postnatal Development			
Neurotoxicity		**LOW: Tris(tribromophenoxy) triazine is expected to have limited bioavailability. It is estimated to have low potential for neurotoxicity based on professional judgment.**		
	Neurotoxicity Screening Battery (Adult)	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2011	Based on SF discrete organic chemicals assessment guidance.

Tris(tribromophenoxy) Triazine CASRN 25713-60-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Repeated Dose Effects		**LOW: Tris(tribromophenoxy) triazine is expected to have limited bioavailability. It is estimated to have low potential for repeated dose effects based on professional judgment. Results from a 28-day repeated dose study are consistent with this low concern for toxicity.**		
		Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2011	Based on SF discrete organic chemicals assessment guidance.
		In a 28-day repeated dose study, rats (6/sex) were orally exposed to 0, 10, 50, 250, or 1,000 mg/kg bw-day. There was neither mortality nor treatment-related clinical signs of toxicity. There was a decreased reticulocyte count and relative adrenal weight in females and increased relative liver weight and decreased relative kidney weight in males; however, these effects were not considered dose- or treatment-related. NOAEL = 1,000 mg/kg bw/day (highest dose tested)	NICNAS, 2006	Reported in a secondary source.
Skin Sensitization		**LOW: Tris(tribromophenoxy) triazine was not a skin sensitizer in one study of guinea pigs.**		
	Skin Sensitization	Negative results in a skin sensitization maximization test in guinea pigs (0–6% response rate).	NICNAS, 2006	Reported in a secondary source.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Tris(tribromophenoxy) triazine was a slight eye irritant in one study of rabbits.**		
	Eye Irritation	Slightly irritating to rabbit eyes	NICNAS, 2006	Reported in a secondary source.
Dermal Irritation		**VERY LOW: Tris(tribromophenoxy) triazine was not a skin irritant in one study of rabbits.**		
	Dermal Irritation	Non-irritating to rabbit skin	NICNAS, 2006	Reported in a secondary source.
Endocrine Activity		**Tris(tribromophenoxy) triazine is expected to have limited bioavailability. It is estimated to have low potential for endocrine activity based on professional judgment.**		

Tris(tribromophenoxy) Triazine CASRN 25713-60-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2011	Based on SF discrete organic chemicals assessment guidance.
Immunotoxicity		**Tris(tribromophenoxy) triazine is expected to have limited bioavailability. It is estimated to have low potential for immunotoxicity based on professional judgment.**		
	Immune System Effects	Limited bioavailability expected (Estimated)	Professional judgment; EPA, 2011	Based on SF discrete organic chemicals assessment guidance.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**LOW: Tris(tribromophenoxy) triazine is expected to display no effects at saturation (NES) because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.**		
Fish LC_{50}		NES	Professional judgment	The MW >1,000, limited bioavailability and low water solubility suggest there will be NES.
Daphnid LC_{50}		NES	Professional judgment	The MW >1,000, limited bioavailability and low water solubility suggest there will be NES.
Green Algae EC_{50}		NES	Professional judgment	The MW >1,000, limited bioavailability and low water solubility suggest there will be NES.
Chronic Aquatic Toxicity		**LOW: Tris (tribromophenoxy) triazine is expected to display NES because the amount dissolved in water is not anticipated to reach a concentration at which adverse effects may be expressed.**		
Fish ChV		NES	Professional judgment	The MW >1,000, limited bioavailability and low water solubility suggest there will be NES.
Daphnid ChV		NES	Professional judgment	The MW >1,000, limited bioavailability and low water solubility suggest there will be NES.

Tris(tribromophenoxy) Triazine CASRN 25713-60-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Green Algae ChV		NES	Professional judgment	The MW >1,000, limited bioavailability and low water solubility suggest there will be NES.
ENVIRONMENTAL FATE				
Transport		**The transport assessment for tris(tribromophenoxy) triazine is based almost entirely on behavior anticipated for high MW (>1,000), water insoluble, nonvolatile materials. Leaching of tris(tribromophenoxy) triazine through soil to groundwater is not expected to be an important transport mechanism. Estimated volatilization half-lives indicate that it will be nonvolatile from surface water. Volatilization from dry surface is also not expected based on its vapor pressure. In the atmosphere, this compound is expected to exist solely in the particulate phase, based on its estimated vapor pressure. Particulates may be removed from air by wet or dry deposition.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	EPI; Professional judgment	Although this material may be outside the MW domain for the estimation model, the resulting value is consistent with that anticipated for a highly brominated, high MW substance. Cutoff value used for non volatile compounds.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	>30,000 (Estimated)	EPI; EPA, 2011	Although this material may be outside the MW domain for the estimation model, the resulting value is consistent with that anticipated for a highly brominated, high MW substance. Cutoff value for non mobile compounds according to SF assessment guidance.

Tris(tribromophenoxy) Triazine CASRN 25713-60-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Level III Fugacity Model	Air = <1% (Estimated) Water = 4.2% Soil = 93% Sediment = 2.8%	EPI	Although this material may be outside the MW domain for the estimation model, the resulting value is consistent with that anticipated for a highly brominated, high MW substance.
Persistence		**VERY HIGH: Biodegradation is not expected to be a major removal process based on experimental data. No biodegradation occurred in a 28-day ready biodegradation test. In a guideline inherent biodegradation test, only 4% of the test substance was removed in 72 days. Therefore, biodegradation is not expected to be a major removal process. Volatilization, atmospheric photooxidation, and hydrolysis are also not expected to occur. Therefore, tris(tribromophenoxy) triazine is expected to be highly persistent in the environment.**		
Water	**Aerobic Biodegradation**	Not readily biodegradable after 28 days; no degradation measured by BOD using microorganisms obtained from activated sludge, 6% measured by HPLC (Measured)	NICNAS, 2006	Adequate; value reported in a secondary source.
		Not inherently biodegradable after 72 days; 4% degradation according to OECD 302D (Measured)	NICNAS, 2006	Adequate; value reported in a secondary source.
		Recalcitrant (Estimated)	EPI; Professional judgment	Although this material may be outside the MW domain for the estimation model, the resulting value is consistent with that anticipated for a highly brominated, high MW substance.
		Not probable (Anaerobic-methanogenic biodegradation probability model)	EPI; Professional judgment	Although this material may be outside the MW domain for the estimation model, the resulting value is consistent with that anticipated for a highly brominated, high MW substance.

Tris(tribromophenoxy) Triazine CASRN 25713-60-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Volatilization Half-life for Model River	>1 year (Estimated)	EPI; Professional judgment	Although this material may be outside the MW domain for the estimation model, the resulting value is consistent with that anticipated for a highly brominated, high MW substance.
	Volatilization Half-life for Model Lake	>1 year (Estimated)	EPI; Professional judgment	Although this material may be outside the MW domain for the estimation model, the resulting value is consistent with that anticipated for a highly brominated, high MW substance.
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation			No data located.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	Not a significant fate process (Estimated)	Professional judgment	This chemical is expected to exist in the particulate phase in the atmosphere.
Reactivity	**Photolysis**			No data located.
	Hydrolysis	Not a significant fate process (Estimated)	Boethling and Mackay, 2000; Professional judgment	The substance does not contain functional groups that would be expected to hydrolyze and has negligible water solubility.

Tris(tribromophenoxy) Triazine CASRN 25713-60-4				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Environmental Half-life		>180 days (Estimated)	EPI; Professional judgment	Although this material may be outside the MW domain for the estimation model, the resulting value is consistent with that anticipated for a highly brominated, high MW substance.
Bioaccumulation		**HIGH: The estimated BAF for this chemical is >5,000. Although measured BCF values were located, estimated BAF values are incorporated for a conservative approach. The BAF estimate is consistent with the potential for bioaccumulation that is anticipated for high MW chemicals with a high degree of bromination.**		
	Fish BCF	<0.8 to 9; <8 to 18 (*Oryzias latipes*) (Measured) Using continuous flow-through test	NICNAS, 2006	Results are consistent with chemicals with low water solubility and high MW, suggesting limited transport through gills.
	BAF	8,800 (Estimated)	EPI	Although this material may be outside the MW domain for the estimation model, the resulting value is consistent with that anticipated for a highly brominated, high MW substance. Assessment criteria indicate estimated BAF may be used in preference to measured BCF values.
	Metabolism in Fish			No data located.

Tris(tribromophenoxy) Triazine CASRN 25713-60-4			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
ENVIRONMENTAL MONITORING AND BIOMONITORING			
Environmental Monitoring	No data located.		
Ecological Biomonitoring	No data located.		
Human Biomonitoring	This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

Boethling, R., Mackay, D. *Handbook of Property Estimation Methods for Chemicals, Environmental Health Sciences*. Boca Raton: Lewis Publishers. **2000**.

CDC (Centers for Disease Control and Prevention). *Fourth national report on human exposure to environmental chemicals, updated tables*. Department of Health and Human Services. **2011.** http://www.cdc.gov/exposurereport/pdf/Updated_Tables.pdf (accessed on May 10, 2011).

EPA Sustainable Futures. *Using NonCancer Screening within the SF Initiative.* Environmental Protection Agency: Washington D.C. **2011a.** http://www.epa.gov/opptintr/sf/pubs/noncan-screen.htm#systemic (accessed on February 09, 2011).

[SF Assessment Guidance] EPA (Environmental Protection Agency). Sustainable Futures Summary Assessment. *Assessment of Discrete Organic Chemicals*. U.S. Environmental Protection Agency: Washington D.C. **2011b**. http://www.epa.gov/oppt/sf/pubs/iad_discretes_092011.pdf

[HPV Assessment Guidance] EPA (Environmental Protection Agency). *Determining the Adequacy of Existing Data.* U.S. Environmental Protection Agency: Washington D.C. **1999.** http://www.epa.gov/hpv/pubs/general/datadeqfn.pdf

EPI *(EPIWIN/EPISUITE) Estimations Programs Interface for Windows*, Version 4.0. U.S. Environmental Protection Agency: Washington D.C. http://www.epa.gov/opptintr/exposure/.

NICNAS Full Study Report, File No:STD/1132, **2006.** http://www.nicnas.gov.au/publications/car/new/std/stdfullr/std1000fr/std1132fr.pdf (accessed on April 11, 2011).

Pakalin, S.; Cole, T.; Steinkellner, J.; Nicolas, R.; Tissier, C.; Munn, S.; Eisenreich, S. Review on Production Processes of Decabromodiphenyl Ether (DECABDE) used in Polymeric Applications in Electrical and Electronic Equipment, and Assessment of the Availability of Potential Alternatives to DECABDE. [Online] **2007**. http://publications.jrc.ec.europa.eu/repository/handle/111111111/5259 (accessed on January 20, 2011).

Zinc Borate

Screening Level Hazard Summary

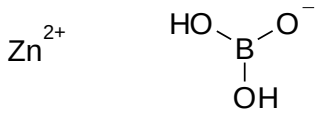
This table only contains information regarding the inherent hazards of flame retardant chemicals. Evaluation of risk considers both the hazard and exposure associated with a substance including combustion and degradation byproducts. The caveats listed in the legend and footnote sections must be taken into account when interpreting the hazard information in the table below.

VL = Very Low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very High hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on empirical data. Endpoints in black italics *(VL, L, M, H,* and *VH*) were assigned using values from estimation software and professional judgment.

[R] Recalcitrant: substance is or contains inorganics, such as metal ions or elemental oxides, that are expected to be found in the environment >60 days after release

		Human Health Effects										Aquatic Toxicity		Environmental Fate	
Chemical	CASRN	Acute Toxicity	Carcinogenicity	Genotoxicity	Reproductive	Developmental	Neurological	Repeated Dose	Skin Sensitization	Respiratory Sensitization	Eye Irritation	Dermal Irritation	Acute	Chronic	Persistence	Bioaccumulation
Zinc Borate	1332-07-6	L	*L*	*H*	*M*	*M*	*H*	*L*	L		L	L	*H*	*H*	H [R]	*L*

Zinc Borate



CASRN: 1332-07-6, 138265-88-0

MW: 125

MF: $ZnBO_3H$ (Empirical)

Physical Forms:
Neat: Solid

Use: Flame retardant

SMILES: Not applicable

Synonyms: Boric acid, zinc salt (TSCA Inventory); Boron zinc hydroxide oxide; Alcanex FR 100; Alcanex FRC 600; Bonrex FC; Borax 2335; Borogard ZB; Climax; ZB 467; 128859; FRC 600; Firebrake 415; Firebrake 500; Firebrake ZB; Flamtard Z 10; JS 9502; SZB 2335; Storshield ZB2335; XPI 187; ZB 112; ZB 113; ZB 223; ZB 237; ZB 325; ZB 467 Lite; ZB-Shield; ZN 100; ZSB 2335; ZT; Zinc borate

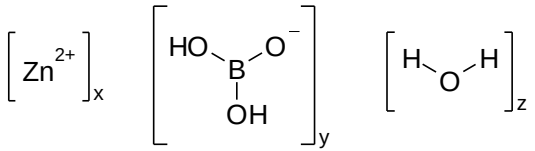
Chemical Considerations: This alternative is an inorganic compound. Zinc borates have the general formula $xZnO \cdot yB_2O_3 \cdot zH_2O$. Zinc borate hydrate analogs may have differing and possibly complex ratios for the water of hydration. In the absence of experimental data, professional judgment using chemical class and structural considerations were used to complete this hazard profile.

Polymeric: No
Oligomers: Not applicable

Metabolites, Degradates and Transformation Products: Zinc (23713-49-7), borate (39201-27-9), zinc oxide (1314-13-2), zinc hydroxide, boric acid (10043-35-3; 11113-50-1)

Analogs: Zinc borate hydrate analogs include CASRNs 12447-61-9, 12513-27-8, 27043-84-1, 12280-01-2, 12429-73-1, 12536-65-1, 147749-62-2 (Briggs, 2004; Smith, 2002; Lide, 2008, Touval, 2000, Goodwin, 2006); analog data from other confidential compounds was also used.
Endpoint(s) using analog values: Not applicable

Analog Structure:



Structural Alerts: Boron containing compounds, developmental toxicity (U.S. EPA, 2011a)

Risk Phrases: R50/53 – Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. Zinc borate's dissolution produces soluble zinc ions (Firebrake MSDS, 2002). Not classified by Annex VI Regulation (EC) No 1272/2008 (ESIS, 2011).

Hazard and Risk Assessments: Risk assessment completed for zinc borate by the National Academy of Sciences in 2000 (NAS, 2000); Pesticide Registration review, EPA (2011).

U.S. EPA TSCA Regulatory Status: 1332-07-6 – This chemical is listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory. 138265-88-0 – This chemical is not listed on the non-confidential Toxic Substances Control Act (TSCA) Inventory.

Zinc Borate CASRN 1332-07-6, 138265-88-0			
PROPERTY/ENDPOINT	**DATA**	**REFERENCE**	**DATA QUALITY**
PHYSICAL/CHEMICAL PROPERTIES			
Melting Point (°C)	980 (for 12513-27-8 and 138265-88-0) (Estimated by analogy)	Lewis, 1993; NAS, 2000; Gowda, 2007; Lide, 2008	The values reported for the zinc borate and its hydrates are consistent with that expected for these inorganic salts, which are characterized by high melting points. At elevated temperatures, the hydrated materials may lose their waters of hydration.
	Phase change at 650 (Measured)	Firebrake MSDS, 2002	
	>550 (for 12447-61-9) (Estimated by analogy)	EPA Factsheet, 1991	
Boiling Point (°C)	>500, Decomposes (Estimated)	Professional judgment	Adequate; decomposition occurs upon melting as described in located sources above. This is anticipated to occur at or above the melting point.
Vapor Pressure (mm Hg)	$<10^{-8}$ (Estimated)	Professional judgment; EPA, 2011b	Cutoff value for nonvolatile materials according to SF assessment guidance; expected for an inorganic salt.
	Negligible (Measured)	HDP, 2004	Qualitative, nonspecific value.
Water Solubility	<0.28% at 25°C (Measured)	Clayton and Clayton, 1994; HDP, 2004; Firebrake MSDS, 2002	The values reported for the zinc borate hydrates indicate that its dissolution is pH dependent and includes the pH range 5-7 that is typically found in the environment.
	0.1% at pH 5 and 7 and 23°C 0.03% at pH 9 and 23°C (for 12447-61-9) (Estimated by analogy)	Lindsay, 1991	
	Zinc borate is slightly soluble in water. At low pH, zinc borate can dissociate to zinc and borate ions (for 12447-61-9) (Estimated by analogy)	Sanders, 2007	Indicates the potential for liberation of zinc ions under acid conditions such as those found in the stomach.
Log K_{ow}			No data located. Compound is not amenable to available estimation techniques.
Flammability (Flash Point)	Nonflammable (Measured)	Sax and Lewis, 1987	Adequate.

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Explosivity		Not explosive (Measured)	Firebreak MSDS, 2002	Adequate.
Pyrolysis		Not applicable (Estimated)	Professional judgment	Inorganic compounds do not undergo pyrolysis.
pH		7.6 (for 12447-61-9) (Estimated by analogy) In a 1%suspension of product to distilled water by mass concentration (w:w).	Gowda, 2007	Adequate; indicates that this substance is a weak base in solution.
pK_a				No data located; inorganic compounds are outside the estimation domain of SPARC.
HUMAN HEALTH EFFECTS				
Toxicokinetics		**Zinc borate is estimated to not be absorbed through skin. Absorption is expected through lungs and gastrointestinal (GI) tract. Limited toxicokinetic data suggest that zinc borate breaks down readily in the stomach to zinc oxide and boric acid.**		
Dermal Absorption *in vitro*				No data located.
Absorption, Distribution, Metabolism & Excretion	**Oral, Dermal or Inhaled**	No exposure expected through skin but absorption expected through lungs and GI tract. (Estimated by analogy)	Professional judgment	Based on closely related confidential analogs with similar structures, functional groups, and physical/ chemical properties.
		Zinc borate readily breaks down to zinc oxide and boric acid in the stomach.	NAS, 2000	Limited study details reported in a secondary source.
Acute Mammalian Toxicity		**LOW: Based on acute toxicity values >2,000 mg/kg for the oral and dermal routes of exposure. Data are inadequate to assess inhalation exposure.**		
Acute Lethality	**Oral**	**Zinc borate:** Rat oral LD_{50} >10,000 mg/kg	EPA, 1991 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
		Zinc borate: Rat oral LD_{50} >5,000 mg/kg	Cervan, 1992 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
		Zinc borate: Rat oral LD_{50} >10,000 mg/kg	Daniels et al., 1969 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
	Dermal	**Zinc borate:** Rabbit dermal LD_{50} >10,000 mg/kg	EPA, 1991 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
	Inhalation	**Zinc borate:** (species unspecified) inhalation LC_{50} >5 mg/L	EFRA, 2006 Weir	Inadequate; no study details reported in a secondary source. Species not identified; not specified if aerosol or dust/fume form.
Carcinogenicity		**LOW: There is no evidence of carcinogenicity following exposure to zinc borate or its metabolites zinc oxide and boric acid. Zinc borate is not listed as a known carcinogen by IARC, NTP, U.S. EPA or California Proposition 65.**		
	OncoLogic Results			No data located.
	Carcinogenicity (Rat and Mouse)	**Zinc borate:** Not listed as a known carcinogen by IARC, NTP, U.S. EPA, or California Proposition 65.	Maine DEP, 2007	Limited study details reported in a secondary source.
		Boric acid: 2-year feeding study in rats and dogs. No carcinogenic effects observed in either rats or dogs at doses as high as 58.5 and 40.8 mg/kg-day, respectively.	Weir and Fisher, 1972 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
		Boric acid: No carcinogenic effects reported in mice exposed to doses as high as 201 mg/kg-day in an NTP bioassay.	NTP, 1987 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
	Combined Chronic Toxicity/ Carcinogenicity			No data located.
Genotoxicity		**HIGH: Potential for mutagenicity based on exposure to zinc. Zinc borate did not cause gene mutations or chromosomal aberrations *in vitro*. In addition, *in vitro* and *in vivo* assays for the metabolite boric acid were negative for genotoxicity.**		
	Gene Mutation *in vitro*	**Zinc:** Potential for mutagenicity based on exposure to zinc (Estimated)	Professional judgment	Estimated based on professional judgment.
		Zinc borate: Ames assay in *Salmonella typhimurium*: Negative with and without metabolic activation	EPA, 1991 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Boric acid: Mutation assays in *S. typhimurium, Escherichia coli*, and mammalian cells (L5178Y mouse lymphoma, V79 Chinese hamster cells, C3H/10T1/2 cells): Negative	Haworth et al., 1983; Landolph, 1985; NTP, 1987; Bakke, 1991; Stewart, 1991 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
	Gene Mutation *in vivo*	**Boric acid:** *In vivo* mouse bone marrow micronucleus assay: Negative	O'Loughlin, 1991 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
	Chromosomal Aberrations *in vitro*	**Zinc borate:** Did not induce chromosomal aberrations *in vitro*: Negative	EPA, 1991 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
		Boric acid: Chromosomal aberration and sister chromatid exchanges in mammalian cells (CHO): Negative	Haworth et al., 1983; Landolph, 1985; NTP, 1987; Bakke, 1991, Stewart, 1991(as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
	Chromosomal Aberrations *in vivo*			No data located.
	DNA Damage and Repair	**Boric acid:** Negative in bacterial DNA-damage assay, unscheduled DNA synthesis in hepatocytes	Haworth et al., 1983; Landolph, 1985; NTP, 1987; Bakke, 1991, Stewart, 1991 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
	Other (Mitotic Gene Conversion)			No data located.

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Reproductive Effects		**MODERATE: Estimated based on reproductive system effects following exposure to boric acid. Exposure to boric acid resulted in male reproductive toxicity including increased incidence of testicular atrophy, reduced sperm count, and degeneration of seminiferous tubules.**		
	Reproduction/ Developmental Toxicity Screen	**Boric acid:** Rat 3-generation study; increased incidence of testicular atrophy, degeneration of seminiferous tubules, reduced sperm count and reduced fertility. NOAEL = 17.5 mg boron/kg-day (corresponding to 100 mg boric acid/kg-day) LOAEL = 58.5 mg boron/kg-day (corresponding to 334 mg boric acid/kg-day)	Weir and Fisher, 1972 (as cited in Maine DEP, 2007)	Study details reported in a secondary source.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Reproduction and Fertility Effects	**Boric acid:** Increased incidence of reversible disruption of tubular spermiation in rats administered 175 mg/kg-day LOAEL = 175 mg/kg-day	Linder et al., 1990 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
		Boric acid: No reproductive effects reported in rats following exposure to a single dose of 2,000 mg/kg-day NOAEL = 2,000 mg/kg-day	Bouissous and Castagnol, 1965 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
		Boric acid: Increased incidence of reversible inhibition of spermiation in rats administered 217 mg/kg-day for 14 days LOAEL = 217 mg/kg-day	Ku et al., 1993 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Developmental Effects		**MODERATE: Estimated based on developmental effects following exposure to zinc oxide, known to be formed from zinc borate in the stomach. Exposure to zinc oxide resulted in increased incidence of stillborn pups. Developmental toxicity data for boric acid exposure in rabbits, rats and mice are consistent with this hazard designation.**		
	Reproduction/ Developmental Toxicity Screen			No data located.
	Combined Repeated Dose with Reproduction/ Developmental Toxicity Screen			No data located.
	Prenatal Development	**Zinc oxide:** Rat, oral (diet) exposure from GD 0 to LD 14; no external malformations were observed. There were no effects on maternal weight, daily food intake, duration of gestation and number of viable young/litter decreased pup dry liver weights. There were 4 stillborn pups (not edematous) in dams of rats exposed to 150 mg/kg-day and 2 females had stillborn litters containing edematous pups in rats exposed to 375 mg/kg-day. LOAEL= 150 mg ZnO/kg-day	Ketcheson et al. 1969 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Boric acid: Rabbit; GD 6-19, oral (gavage); developmental effects. Rabbit: Maternal and Developmental NOAEL = 125 mg/kg-day Maternal and Developmental LOAEL = 250 mg/kg-day Rat: NOAEL = 78 mg/kg-day Mouse: NOAEL= 248 mg/kg- day	U.S. Borax and Chemical Corp, 1992a.	Limited study details reported; TSCATS submission.
	Postnatal Development			No data located.
Neurotoxicity		**HIGH: Estimated based on analogy to data for boric acid. Limited data indicate a 4-hour inhalation exposure to boric acid may cause neurotoxic effects in rats at 0.16 mg/L. Limited data were located regarding neurotoxic effects caused by exposure to zinc borate or zinc oxide. There is also potential for developmental neurotoxicity based on boric acid using expert judgment.**		
	Neurotoxicity	**Boric acid:** Rat 4-hour dust inhalation; caused reduced righting reflex, hunched posture, lacrimation and rales LOAEL = 0.16 mg/L	U.S. Borax and Chemical Corp., 1992b	Limited study details reported; TSCATS submission.
		Boric acid: Potential for developmental neurotoxicity (Estimated)	Expert judgment	Estimated based on expert judgment.
		Zinc borate: Not classified as a developmental neurotoxicant.	Grandjean and Landrigan, 2006 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
		Zinc borate: Not listed as a potential neurotoxicant on the Red List of Chemicals	CPA, 2009 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Zinc oxide: Rat, 10-day gavage exposure; degenerative changes and histoenzymatic changes, degenerative changes of neurocytes, accompanied with proliferation of the oligodendroglia, and glial proliferation in the white matter. Histoenzymatic changes including decreased ACP, ATPase, AChE, BChE activity and increased TTPase and NSE activity.	Kozik et al., 1980 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
Repeated Dose Effects		**LOW: Estimated based on data for boric acid. Limited data indicate repeated exposure to boric acid may cause effects including decreased food consumption and body weight gain, clinical signs of toxicity and changes in hematological parameters, though these effects occur at doses of >100 mg/kg-day of boric acid. No repeated dose toxicity data were located for zinc borate.**		
		Zinc oxide: Ferrets; oral (feed) 21-day exposure; pale livers with fatty infiltration and enlarged kidneys; macrocytic hypochromic anemia, increased reticulocytes and leucocytosis. Increased severity at higher doses. NOAEL = 81.3 mg/kg-day LOAEL = 243.8 mg/kg-day	Straube et al., 1980 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
		Boric acid: 2-year feeding study in rats and dogs; effects in rats included decreased food consumption and body weight gain, course hair coats, hunched position, swollen pads, inflamed bleeding eyes and changes in hematological parameters. Diarrhea and soft stool was observed in dogs. Testicular effects were reported for both rats and dogs. NOAEL = 100 mg boric acid/kg-day LOAEL = 334 mg boric acid/kg-day	Weir and Fisher, 1972 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source. Values from primary source are reported as boron equivalent doses. Doses as boric acid were not reported but are calculated by dividing the boron equivalent doses with the MW of boric acid (0.1750). i.e., NOAEL = 17.5 mg boron/kg-day (corresponding to 100 mg boric acid/kg-day) LOAEL = 58.5 mg boron/kg-day corresponding to 334 mg boric acid/kg-day)
Skin Sensitization		**LOW: Zinc borate is not a skin sensitizer in guinea pigs.**		
	Skin Sensitization	**Zinc borate:** Not a skin sensitizer in guinea pigs	U.S. Borax, 1996 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
		Boric acid: Not a skin sensitizer in humans or animals	Wnorowski, 1994a,b,c; Bruze et al., 1995 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
Respiratory Sensitization		**No data located.**		
	Respiratory Sensitization			No data located.
Eye Irritation		**LOW: Zinc borate causes no irritation to mild irritation.**		
	Eye Irritation	Contact with eyes causes irritation	HSDB, 2011	Limited study details reported in a secondary source.
		Mild conjunctivitis; not considered to be and eye irritant or corrosive, rabbit	U.S. Borax, 1996 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.
		Eye irritant with mild conjunctivitis, rabbit	EPA, 1991 (as cited in Maine DEP, 2007)	Limited study details reported in a secondary source.

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Dermal Irritation		**LOW: Zinc borate may cause skin irritation, but is not corrosive.**		
	Dermal Irritation	Contact with skin causes irritation	HSDB, 2011	No study details reported in a secondary source.
		Not irritant or corrosive	EPA, 1991 (as cited in Maine DEP, 2007)	No study details reported in a secondary source.
Endocrine Activity		**Does not have potential for endocrine activity based on expert judgment.**		
		No potential for endocrine activity (Estimated)	Expert judgment	Estimated based on expert judgment.
Immunotoxicity		**There is uncertain potential for immunotoxicity based on exposure to zinc ions.**		
	Immune System Effects	Uncertain potential for immunotoxic effects (Estimated by analogy)	Professional judgment	Based on confidential data to other Zn^{2+} compounds.
ECOTOXICITY				
ECOSAR Class		Not applicable		
Acute Toxicity		**HIGH: Based on estimated potential for dissolved zinc species to cause adverse effects in aquatic species, as described in the EPA Chemical Categories document which includes all soluble complexes of zinc. (Professional judgment)**		
Fish LC_{50}		Potential for adverse effects in aquatic species. (Estimated)	Professional judgment	Estimated based on aquatic toxicity effects from dissolve zinc species as described in the EPA Chemical Categories document.
		Zinc borate: Classified as Dangerous to the Environment, R50/R53, very toxic to aquatic organisms may cause long-term effects in the aquatic environment.	EFRA, 2006 (as cited in Maine DEP, 2007)	Limited study details reported in the database.
		Zinc borate: *Lepomis macrochirus* (bluegill) 96-hour LC_{50} = 335 mg/L	ECOTOX, 2011	Limited study details reported in the database.
		Zinc borate: *Oncorhynchus mykiss* (rainbow trout) 96-hour LC_{50} = 2.7 mg/L	ECOTOX, 2011	Limited study details reported in the database.
Daphnid LC_{50}		**Zinc borate:** *Daphnia magna* 48-hour EC_{50} = 75 mg/L	ECOTOX, 2011	Limited study details reported in the ECOTOX database.
Green Algae EC_{50}				No data located.

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Chronic Aquatic Toxicity		**HIGH: Based on estimated potential for dissolved zinc species to cause adverse effects in aquatic species, as described in the EPA Chemical Categories document which includes all soluble complexes of zinc. (Professional judgment)**		
Fish ChV		Potential for adverse effects in aquatic species. (Estimated)	Professional judgment	Estimated based on aquatic toxicity effects from dissolve zinc species as described in the EPA Chemical Categories document.
		Zinc borate: Classified as Dangerous to the Environment, R50/R53, very toxic to aquatic organisms may cause long-term effects in the aquatic environment.	EFRA, 2006 (as cited in Maine DEP, 2007)	Limited study details reported in the database.
Daphnid ChV				No data located.
Green Algae ChV				No data located.
ENVIRONMENTAL FATE				
Transport		**The transport evaluation for zinc borate is based on located experimental and estimated physical/chemical properties. The low water solubility, low vapor pressure (10^{-8}), estimated high soil adsorption and Henry's Law Constant ($<10^{-8}$) indicate that zinc borate will be relatively immobile in the environment. Transport is more likely to occur in water and at low pH, where zinc borate dissociates into zinc and borate ions.**		
	Henry's Law Constant (atm-m^3/mole)	$<10^{-8}$ (Estimated)	Professional judgment	Cutoff value for nonvolatile compounds such as inorganic salts. This inorganic compound is not amenable to available estimation methods.
	Sediment/Soil Adsorption/Desorption Coefficient – K_{oc}	Zinc borate is sparingly soluble in water and is not expected to leach through soil. (Estimated)	Professional judgment	Available methods for estimating K_{oc} values cannot be directly applied to inorganic salts.
	Level III Fugacity Model			Not all input parameters for this model were available to run the estimation software (EPI).

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Persistence		**HIGH: Zinc borate is expected to have high persistence in the environment because of the persistence of Zn^{2+} ions. The behavior of zinc borate in water is complex. In acidic aqueous conditions zinc borate releases Zn^{2+} and boric acid; the Zn^{2+} will not undergo further degradation (but can undergo precipitation, sorption, or ligand exchange reactions in the environment). In basic aqueous conditions, zinc borate forms boric acid and hydrated zinc oxide. Zinc borate was found to be stable in sunlight, under normal and elevated temperatures, according to an EPA guideline study.**		
Water	**Aerobic Biodegradation**			No data located.
	Volatilization Half-life for Model River			No data located.
	Volatilization Half-life for Model Lake			No data located.
Soil	**Aerobic Biodegradation**			No data located.
	Anaerobic Biodegradation			No data located.
	Soil Biodegradation with Product Identification			No data located.
	Sediment/Water Biodegradation			No data located.
Air	**Atmospheric Half-life**	>1 year (Estimated)	Professional judgment	Substance is or contains inorganic elements such as metal ions or oxides that are not amenable to atmospheric degradation processes.
Reactivity	**Photolysis**	Stability to sunlight, normal and elevated temperature, according to EPA Method 830.6313 for metals/metal ions (for 12447-61-9) (Estimated by analogy)	Gowda, 2007	Adequate; guideline study.
	Hydrolysis	<10 minutes at pH 6 48 hours at pH 9 (for 12447-61-9) (Estimated by analogy)	Lords, 2007	Adequate; formation of insoluble hydrated zinc oxide precipitate occurs at a pH of 9.

Zinc Borate CASRN 1332-07-6, 138265-88-0				
PROPERTY/ENDPOINT		**DATA**	**REFERENCE**	**DATA QUALITY**
Environmental Half-life				Not all input parameters for this model were available to run the estimation software (EPI).
Bioaccumulation		**LOW: Zinc borate is not expected to be very soluble in water and therefore does not have potential for bioaccumulation.**		
	Fish BCF	<100 (Estimated)	Professional judgment	This inorganic compound is not amenable to available estimation methods.
	BAF	<100 (Estimated)	Professional judgment	This inorganic compound is not amenable to available estimation methods.
	Metabolism in Fish			No data located.
ENVIRONMENTAL MONITORING AND BIOMONITORING				
Environmental Monitoring		No data located.		
Ecological Biomonitoring		No data located.		
Human Biomonitoring		This chemical was not included in the NHANES biomonitoring report (CDC, 2011).		

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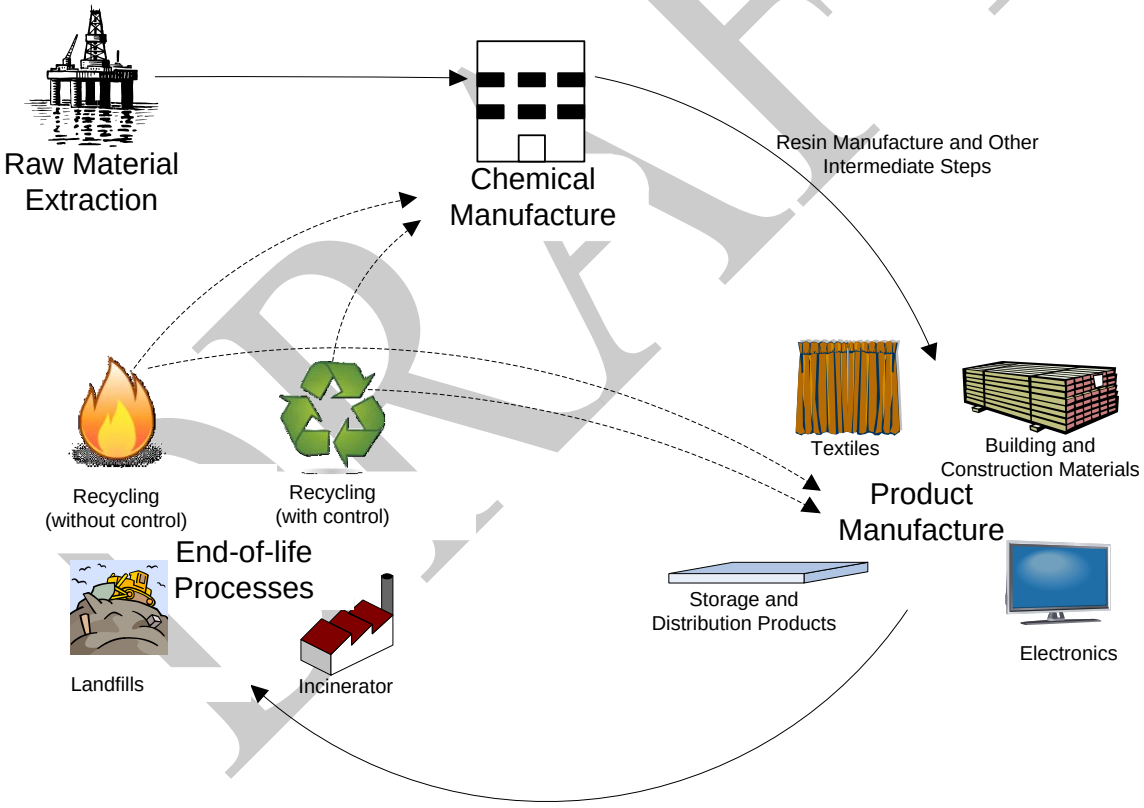
5 General Exposure Information and Other Life-Cycle Considerations

The purpose of this chapter is to provide general information on exposure and life-cycle considerations for flame retardant chemicals. Section 5.1 includes an overview of exposure considerations and also includes data on some of the physical-chemical properties which impact the probability of exposure to decaBDE and the alternatives included in the assessment. A quantitative exposure assessment is outside the scope of this project and is not necessary for a comparative hazard assessment. This discussion is framed in the context of five life-cycle stages: extraction (Section 5.2), chemical manufacture (Section 5.3), product manufacture (Section 5.4), product use (Section 5.5) and end-of-life (Section 5.6), as shown in Figure 5-1. Depending on the product type, intermediate steps between chemical and product manufacturing may be relevant; these are briefly discussed in Section 5.4. The chapter is intended to help the reader understand the factors that affect exposure to decaBDE and alternative flame retardants across the life-cycle.

Figure 5-1: Life Cycle Stages Included in this Chapter



5.1 Potential Exposure Pathways and Routes (General)

Exposure can occur at many points in the life cycle of a flame retardant chemical. Occupational exposures may occur during raw material extraction, chemical and product manufacturing and at product end-of-life (i.e., reuse, refurbishing, recycling, incinerating or landfilling). Consumers may be exposed while the flame retarded product is being used. Exposures to the general

population and environment may result from product manufacturing, use, storage, and end-of-life processes.

The risk associated with a given chemical or substance is influenced by how the exposure occurs. For example, the risk associated with inhaling a chemical can be different from the risk due to ingestion of the same chemical. As a result, exposure is typically characterized by pathway and route. An exposure pathway is the physical course a chemical takes from the source of release to the organism that is exposed. The exposure route is how a chemical gets inside the organism. The three primary routes of exposure are inhalation, dermal absorption, and ingestion. Each chemical's specific physical-chemical properties influence pathways and routes of exposure.

5.1.1 Occupational versus General Population Exposures

Exposures to the general population are different from exposures to workers and should be evaluated separately. Occupational exposures may be both acute and chronic because of direct contact with chemicals at relatively high concentrations while workers are conducting specific tasks such as manufacturing and processing of chemicals. However, certain occupations such as firefighting may result in unique occupational exposure scenarios. It may be more likely for consumers to be exposed chronically, over a long period, but to chemicals incorporated into products or released to the environment from a manufacturing facility. Information on sources of human exposure to decaBDE can be found in Section 5.1.5.

5.1.2 Inhalation Exposures

The physical state of the chemical during chemical manufacturing, downstream processing, incorporation into consumer products, and after release to the environment significantly influences the potential for inhalation exposure. In particular, there are three types of inhalation exposures that may be relevant for evaluation: dust, vapor, and/or mist.

Dust: **"**Dust is defined as solid particles of a substance or mixture suspended in a gas (usually air)" (United Nations 2011). Chemicals that are manufactured, processed, stored, or used as solids, have the potential to result in fugitive dust which may result in occupational exposures. The potential for fugitive dust formation depends on whether the solid chemical is handled in the crystalline form, as an amorphous solid, or as a fine powder. The particle size distribution and handling techniques can also impact the potential for fugitive dust. It is important to note the physical state of the chemical at the potential point of release and contact. For example, the pure chemical may be manufactured as a solid powder, indicating a potential occupational exposure to dust, but it may be formulated into solution before the majority of people come in contact with it, thereby eliminating inhalation exposure to dust as a possible exposure route. The material safety data sheet (MSDS) and best practice should inform the occupational worker when inhalation exposure to the chemical is likely to occur and what respiratory safety measures should be used. Furthermore, there is potential for a chemical to be released from a manufacturing facility and enter a home either through air, dirt or dust. For example, dirt or dust from a workplace may enter a home on a worker's clothing and be subsequently inhaled by other members of the household. Additionally, certain chemicals may be released from a product during consumer use and become incorporated into indoor dust. Consumer exposures are dependent on how a chemical is incorporated into a product and on the chemical's physical-chemical properties.

If there is exposure to dust, particle size influences the degree to which the chemical enters the lungs. Particles less than 10 microns in diameter are "respirable" with potential to reach and attach to tissues in the respiratory tract and deep lung where they may be absorbed into the body. Once released into air or other media, the chemical can associate with particulate material through sorption onto particles or as particulates. For example, vapor phase chemicals can partition onto house dust and contribute to ingestion and dermal exposure pathways as well as inhalation.

Design of transfer facilities, engineering controls, and the use of personal protective equipment will have a greater impact on exposure potential in industrial settings than the size of the dust particles. However, the size of the particles in a manufacturing setting can be considered by individual decision-makers. Compounders may specify that the neat flame retardant be produced in a way that minimizes the low particle size fraction. Although manufacturer-specific, the particle size of the flame retardant chemical can be screened to remove the fine material that can then be returned to the manufacturing process. In residential settings, the flame retardants in electrical equipment and furniture, for example, may migrate to the surface of a material and escape from the polymer matrix, then likely becoming part of house dust. Exposure to flame retardants in house dust can be reduced by dusting frequently and using a vacuum cleaner with a HEPA filter.

Vapor: Vapor is defined as "the gaseous form of a substance or mixture released from its liquid or solid state" (United Nations 2011). Exposure to vapors can occur when chemicals volatilize during manufacturing, processing, storage, and use or are associated with particulates in air. Most chemical manufacturing operations occur in closed systems. However, fugitive emissions are expected during open mixing operations, transfer operations, and loading/unloading of raw materials. The more volatile the chemical the greater the fugitive releases and the higher occupational exposures are likely to be. Therefore, vapor pressure (a measure of volatility) is a key indicator of potential occupational exposures to vapors. Particulate exposures can result from the physical breakdown of products, erosion of materials from surfaces or other similar processes..

Mist: Mist is defined as "liquid droplets of a substance or mixture suspended in a gas (usually air)" (United Nations 2011). Both volatile and non-volatile liquids can result in inhalation exposure if manufacturing or use result in the formation of mist. Particle size is an important consideration in determining exposure to chemicals released as a mist. However, it is unlikely that flame retardant chemicals will be dispersed as a mist.

5.1.3 Dermal Exposures

Dermal exposure is also affected by the physical state of the chemical at the point of release and contact. Additionally, studies have shown that the amount of a chemical that is absorbed through the skin is dependent on where on the body the exposure occurs (U.S. EPA 1992). Dermal exposure is generally assumed to be proportional to the concentration of chemical in the formulation (an exception would be if the solution contains ingredients that enhance dermal transfer). For example, the dermal exposure from contacting a pure chemical is greater than the exposure from contacting a solution that contains only 10 percent of the chemical In addition to

chemical concentration, the extent to which skin will absorb a chemical that it has to come in contact with depends on the chemical's lipophilicity, solubility, polarity volatility, structure and state (e.g., liquid, solid) (U.S. EPA 1992). To be successfully absorbed, compounds must be able to diffuse across both the aqueous pathways and lipid pathways in the skin. To do this, a chemical must first dissolve into the stratum corneum, a stable lipid barrier that is the outermost layer of the skin and the water-based portions of the skin and into the body, which is also water-based (U.S. EPA 2007a). Therefore, the best skin penetrants are "those that exhibit fat- and water-solubility and low levels of crystallinity" (p. 35 U.S. EPA 1992). Dermal exposure to volatile substances is unlikely to occur.

For occupational exposures, screening-level evaluations of dermal exposure can be based on the worker activities involving the chemical. For example, there may be exposure when workers handle bags of solid materials during loading and transfer operations. Maintenance and cleanup activities during shutdown procedures, connecting transfer lines, and sampling activities also result in potential for dermal exposures. For consumers, dermal exposure can occur if a chemical is released from a product that a consumer is handling or is in dust to which an individual comes into contact. Children may have higher dermal exposure because they crawl, roll, or sit on surfaces treated with chemicals and play with objects where residues may settle (U.S. EPA 2008a). However, as stated above, absorption of a chemical through the skin is dependent on the properties of the chemical (U.S. EPA 1992).

5.1.4 Ingestion Exposures

Exposures via ingestion typically occur unintentionally when individuals eat food or drink water that has become contaminated with chemicals or ingest dust on hands. Several pathways should be considered. In regards to occupational exposures, often the primary pathway is poor worker hygiene (eating, drinking, or smoking with unwashed hands.) Additionally, dust particles may spread throughout the facility and settle (or deposit) on tables, lunchroom surfaces, or even on food itself. Vapors may similarly spread throughout the facility and may deposit near food or drinks. Another potential pathway for ingestion occurs from dust particles that are too large to be absorbed through the lungs. These "non-respirable particles" can be swallowed, resulting in exposures from this route. Consumers in the general population may also be exposed through ingestion if a chemical is released from a product and incorporated into dust, which can get on hands or deposit on food and thus be consumed inadvertently. This is an important route of exposure for children, particularly infants and toddlers, who may ingest dust and soil through repeated hand-to-mouth behavior (U.S. EPA 2008a). Compared to inhalation and dermal exposures, ingestion is typically considered a less significant exposure pathway from an occupational health standpoint. However, ingestion can be an equally or more significant exposure pathway for the general population, especially children's ingestion of house dust, than inhalation and dermal exposures.

5.1.5 Human and Environmental Exposure to DecaBDE

This section summarizes the literature on occupational, consumer and environmental exposures to decaBDE. This information on decaBDE exposure can be instructive. Similar patterns of exposure may occur for alternative chemicals. However, exposure information and data are limited and only available for some of the alternatives (Stapleton, Allen et al. 2008; Betts 2009;

Dodge, Pollock et al. 2009; Petito Boyce, Sax et al. 2009; Luo, Chen et al. 2010). Information on products and materials in which decaBDE has been used can be found in Chapter 2.

Human Exposures

According to EPA's 2010 exposure assessment of polybrominated diphenylethers (PBDEs), individuals in occupations that would lead to higher exposures to specific congeners have higher concentrations of PBDE congeners in their blood than the general public (U.S. EPA 2010c). Workers involved in the manufacturing or recycling and disposal of products containing PBDE flame retardants have greater exposure to the chemical compared to the general population (Sjodin, Hagmar et al. 1999; Thomsen, Lundanes et al. 2001; Thuresson, Hoglund et al. 2006).

Consumer exposure to decaBDE is possible given that it can be released from common home products and become a component in house dust (Stapleton, Alaee et al. 2004; Takigamie, Suzuki et al. 2008) (for a list of products where decaBDE may be used, refer to Section 2.2). It is also possible that workers exposed to decaBDE may inadvertently carry particles containing the chemical home with them. This may lead to exposure to family members through household dust or direct contact, as has been proven with other hazardous chemicals such as pesticides and lead (Thompson, Coronado et al. 2003; Minnesota Department of Health 2010). DecaBDE has been found in dust within automobiles (Lagalante, Oswald et al. 2009) and automobile air (Mandalakis, Stephanou et al. 2008). The primary route of consumer exposure to decaBDE is through the ingestion of dust or, for infants, ingestion of breast milk, followed by food and water ingestion and dermal absorption (Lorber 2008; Petito Boyce, Sax et al. 2009; U.S. EPA 2010c). Inhalation may also be a relevant route of exposure (U.S. EPA 2010c). Children have higher levels of exposure to decaBDE than do adults (Petito Boyce, Sax et al. 2009) likely due to higher hand to mouth behavior.

Environmental Exposures

Environmental releases of decaBDE can occur during each stage of a product's life cycle, including chemical manufacturing, product manufacturing, product storage and use, and end-of-life handling (European Communities 2002; U.S. EPA 2009a). In general, levels of PBDEs in humans and the environment are higher in North America than in other regions of the world, likely due to their greater use in North America (Trudel, Scheringer et al. 2011).

Empirical and predicted data indicate that all PBDEs (including decaBDE) are highly persistent in the environment (Environment Canada 2006) and decaBDE has been found in high and increasing concentrations in the sediment of lakes, rivers, streams and estuaries (Song, Li et al. 2005; Environment Canada 2006; Illinois Environmental Protection Agency 2006). Additionally, decaBDE has also been measured in ambient atmospheric particulates (Illinois Environmental Protection Agency 2006) and in the Arctic environment, providing evidence that it is subject to long-range transport (Environment Canada 2006).

Laboratory studies demonstrate decaBDE's bioavailability and metabolism in fish (Illinois Environmental Protection Agency 2006). DecaBDE has been detected in some but not all species

of fish studied (Dodder, Strandberg et al. 2002; European Chemicals Bureau 2002; Johnson-Restrepo, Kannan et al. 2005; Environment Canada 2009; Roberts, Noyest et al. 2011). Also, decaBDE has been measured in birds and their eggs (Lindberg, Sellström et al. 2004; Vorkamp, Thomsen et al. 2005) and in mammals including polar bears, seals, marmots and foxes (Christensen, MacDuffee et al. 2005; Illinois Environmental Protection Agency 2006; Voorspoels, Covaci et al. 2006; Environment Canada 2009). Further, terrestrial species tend to have higher levels of decaBDE than aquatic species for both birds (Jaspers, Covaci et al. 2006) and mammals (Christensen, MacDuffee et al. 2005). These observations indicate bioavailability of decaBDE to wildlife and human food sources with potential for bioaccumulation and biomagnification of decaBDE and/or its degradation products.

5.1.6 Physical-Chemical Properties for the Alternatives to DecaBDE included in this Assessment that May Impact Exposure

Table 5-1 highlights key physical-chemical properties that affect the likelihood of exposure along with the physical-chemical property's relevance to exposure. The properties included in the table are: the physical state of the chemical, vapor pressure, water solubility, dispersibility, log K_{ow}, bioaccumulation potential, and persistence. Descriptions of these properties and how they can be used to predict environmental behavior and hazard potential can be found in Section 4.3. More detailed information on the physical, chemical, and fate properties of each flame retardant chemical can be found in the full chemical summary assessments in Section 4.8.

Table 5-1: Key Physical/Chemical and Fate Properties of Flame Retardant Chemicals

Physical State of Chemical (ambient conditions)						
Relevance to exposure: Indicates if a chemical substance is a solid, liquid, or gas under ambient conditions. This is determined from the melting and boiling points. Chemicals with a melting point more than 25°C are considered solid. Those with a melting point less than 25°C and a boiling point more than 25°C are considered liquid and those with a boiling point less than 25°C are considered a gas. Physical state influences potential for dermal and inhalation exposure. For chemicals that exist as a gas, there is generally a potential for direct inhalation but not dermal exposure. For solids, there is potential for the inhalation and ingestion of dust particles and dermal contact. For liquids, there is potential for direct dermal contact but not for direct inhalation of the liquid (except in operations that produce aerosols).						
Decabromodiphenyl Ether	**Aluminum Diethyl-phosphinate**	**Aluminum Hydroxide**	**Ammonium Polyphosphate**	**Antimony Trioxide**	**Bis (hexachlorocyclopentadieno) Cyclooctane**	**Bisphenol A bis-(diphenylphosphate)**
Solid	Solid	Solid	Solid	Solid	Solid	Solid
Brominated Epoxy Resin End-Capped with Tribromophenol	**Brominated Polyacrylate**	**Brominated Polystyrene**	**Confidential Brominated Epoxy Polymer #1**	**Confidential Brominated Epoxy Polymer #2**	**Confidential Brominated Epoxy Polymer Mixture #1**	**Confidential Brominated Epoxy Polymer Mixture #2**
Solid	Solid	Solid	Solid	Solid	Solid	Solid
Confidential Brominated Polymer	**Decabromodiphenyl Ethane**	**Ethylene bis-tetrabromophthalimide**	**Magnesium Hydroxide**	**Melamine Cyanurate**	**Melamine Polyphosphate**	**N-alkoxy Hindered Amine Reaction Products**
Solid	Solid	Solid	Solid	Solid	Solid	Solid
Phosphonate Oligomer	**Polyphosphonate**	**Poly[phosphonate-co-carbonate]**	**Red Phosphorous**	**Resorcinol bis-diphenylphosphate**	**Substituted Amine Phosphate Mixture**	**TBBPA glycidyl ether, TBBPA polymer**
Solid	Solid	Solid	Solid	Solid	Solid	Solid
TBBPA bis (2,3-dibromopropyl ether)	**Triphenyl Phosphate**	**Tris (tribromoneopentyl) Phosphate**	**Tris (tribromo-phenoxy) Triazine**	**Zinc Borate**		
Solid	Solid	Solid	Solid	Solid		

Vapor Pressure (mm Hg) at 25°C (unless otherwise noted)

Relevance to exposure: Indicates the potential for a chemical to volatilize into the atmosphere. If a chemical has a vapor pressure leading to volatilization at room temperature or typical environmental conditions, then the chemical may evaporate and present the potential for inhalation of the gas or vapor. For a DfE chemical alternatives assessment, inhalation exposure is assumed to occur if the vapor pressure is greater than 1 x 10^{-8} mm Hg. A default value of $<10^{-8}$ was assigned for chemicals without data that are anticipated to be non-volatile (this is based on EPA Sustainable Futures assessment guidance (U.S. EPA 2011e).

Decabromodiphenyl Ether	**Aluminum Diethyl phosphinate**	**Aluminum Hydroxide**	**Ammonium Polyphosphate**	**Antimony Trioxide**	**Bis (hexachlorocyclopentadieno) Cyclooctane**	**Bisphenol A bis-(diphenylphosphate)**
3.5×10^{-8} at 21ºC	$<10^{-8d}$	$<10^{-8c}$	$<10^{-8b}$	$<10^{-8}$	$<10^{-8c}$	$<9\times10^{-6a}$
Brominated Epoxy Resin End-Capped with Tribromophenol	**Brominated Polyacrylate**	**Brominated Polystyrene**	**Confidential Brominated Epoxy Polymer #1**	**Confidential Brominated Epoxy Polymer #2**	**Confidential Brominated Epoxy Polymer Mixture #1**	**Confidential Brominated Epoxy Polymer Mixture #2**
$<10^{-8b}$	$<10^{-8b}$	$<10^{-8b}$	$<10^{-8b}$	$<10^{-8b}$	$<10^{-8b}$	$<10^{-8b}$
Confidential Brominated Polymer	**Decabromodiphenyl Ethane**	**Ethylene bis-tetrabromophthalimide**	**Magnesium Hydroxide**	**Melamine Cyanurate**	**Melamine Polyphosphate**	**N-alkoxy Hindered Amine Reaction Products**
$<10^{-6}$	$<7.5\times10^{-7}$	$<10^{-8d}$	$<10^{-8b}$	$<10^{-8d}$	$<10^{-8d}$	$<10^{-8d}$
Phosphonate Oligomer	**Polyphosphonate**	**Poly[phosphonate-co-carbonate]**	**Red Phosphorous**	**Resorcinol bis-diphenylphosphate**	**Substituted Amine Phosphate Mixture**	**TBBPA glycidyl ether, TBBPA polymer**
$<10^{-8b}$	$<10^{-8b}$	$<10^{-8b}$	0.03 at 21°C	1.9×10^{-5} at 20°C	$<10^{-8c}$	$<10^{-8d}$
TBBPA bis (2,3-dibromo-propyl ether)	**Triphenyl Phosphate**	**Tris (tribromoneo-pentyl) Phosphate**	**Tris (tribromo-phenoxy)Triazine**	**Zinc Borate**		
$<10^{-8d}$	$6.28\text{x}10^{-6a}$	$<10^{-8d}$	$<10^{-8d}$	$<10^{-8b}$		

[a] Extrapolated. [b] Estimated based on EPA Sustainable Futures polymer assessment guidance. [c] Estimated based on EPA Sustainable Futures guidance for nonvolatile compounds. [d] Estimated.

Water Solubility (mg/L)

Relevance to exposure: Indicates the potential of a chemical to dissolve in water and form an aqueous solution. Water soluble chemicals present a higher potential for human exposure through the ingestion of contaminated drinking water (including well water). In general, oral ingestion of a chemical with a water solubility less than 10^{-3} mg/L is not expected. Water soluble chemicals are more likely to be transported into groundwater, absorbed through the gastrointestinal tract or lungs, partition to aquatic compartments, and undergo atmospheric removal by rain washout. A water solubility of 10^{-3} mg/L is used for large, high molecular weight non-ionic polymers according to Sustainable Futures Polymer Assessment guidance (U.S. EPA 1999b). A substance with water solubility at or below 10^{-3} mg/L is considered insoluble.

Decabromodiphenyl Ether	Aluminum Diethyl phosphinate	Aluminum Hydroxide	Ammonium Polyphosphate	Antimony Trioxide	Bis (hexachlorocyclopentadieno) Cyclooctane	Bisphenol A bis-(diphenylphosphate)
$<1.00\times10^{-4}$	2.5×10^{3}	1.5 at 20 ˚C	$<10^{-3c}$	14 at 30 ˚C	4.4×10^{-5}	0.389 – 0.462
Brominated Epoxy Resin End-Capped with Tribromophenol	**Brominated Polyacrylate**	**Brominated Polystyrene**	**Confidential Brominated Epoxy Polymer #1**	**Confidential Brominated Epoxy Polymer #2**	**Confidential Brominated Epoxy Polymer Mixture #1**	**Confidential Brominated Epoxy Polymer Mixture #2**
$<10^{-3c}$	$<10^{-3c}$	$<10^{-3c}$	$<10^{-3c}$	$<10^{-3c}$	$<10^{-3c}$	$<10^{-3c}$
Confidential Brominated Polymer	**Decabromodiphenyl Ethane**	**Ethylene bis-tetrabromophthalimide**	**Magnesium Hydroxide**	**Melamine Cyanurate**	**Melamine Polyphosphate**	**N-alkoxy Hindered Amine Reaction Products**
$<10^{-1}$	7.2×10^{-4}	$<10^{-3b}$	1.78 at 20ºC, pH 8.3	2.7 at 20 ˚C	20,000	$<10^{-3a}$
Phosphonate Oligomer	**Polyphosphonate**	**Poly[phosphonate-co-carbonate]**	**Red Phosphorous**	**Resorcinol bis-diphenylphosphate**	**Substituted Amine Phosphate Mixture**	**TBBPA glycidyl ether, TBBPA polymer**
$<0.0015^{b}$	$<0.0015^{b}$	$<10^{-3c}$	$<10^{-3a}$	1.05 at 20°C	$>1\times10^{6b}$	$<10^{-3b}$
TBBPA bis (2,3-dibromo-propyl ether)	**Triphenyl Phosphate**	**Tris (tribromoneo-pentyl) Phosphate**	**Tris (tribromo-phenoxy)Triazine**	**Zinc Borate**		
$<10^{-3b}$	1.9	0.9	$<10^{-3}$	0.28%*		

*The water solubility of zinc borate is expressed as a percentage and is < 0.28% at neutral pH. Its dissolution is pH dependent and will vary within the range 5-7 that is typically found in the environment. Good water solubility data for zinc borate are not available.

[a] Estimated based on EPA HPV assessment guidance. [b] Estimated. [c] Estimated based on EPA Sustainable Futures polymer assessment guidance.

Log K_{ow}

Relevance to exposure: Indicates a chemical's tendency to partition between water and lipids in biological organisms. A high log K_{ow} value indicates that the chemical is more soluble in octanol (lipophilic) than in water, while a low log K_{ow} value means that the chemical is more soluble in water than in octanol. Log K_{ow} can be used to evaluate absorption and distribution in biological organisms, potential aquatic exposure, and potential general population exposure via ingestion. Generally, chemicals with a log $K_{ow} < 4$ are water soluble and bioavailable, chemicals with a log $K_{ow} \geq 4$ tend to bioaccumulate. Chemicals with a high log K_{ow} also tend to bind strongly to soil and sediment. Log K_{ow} cannot be measured for inorganic substances, polymers, and other materials that are not soluble in either water or octanol. This is indicated in the table with "No data".

Decabromodiphenyl Ether	**Aluminum Diethyl phosphinate**	**Aluminum Hydroxide**	**Ammonium Polyphosphate**	**Antimony Trioxide**	**Bis (hexachlorocyclopentadieno) Cyclooctane**	**Bisphenol A bis-(diphenylphosphate)**
6.27	-0.44[a]	No data	No data	No data	>10[a]	>10[a]
Brominated Epoxy Resin End-Capped with Tribromophenol	**Brominated Polyacrylate**	**Brominated Polystyrene**	**Confidential Brominated Epoxy Polymer #1**	**Confidential Brominated Epoxy Polymer #2**	**Confidential Brominated Epoxy Polymer Mixture #1**	**Confidential Brominated Epoxy Polymer Mixture #2**
No data	No data	No data	No data	No data	No data	No data
Confidential Brominated Polymer	**Decabromodiphenyl Ethane**	**Ethylene bis-tetrabromophthalimide**	**Magnesium Hydroxide**	**Melamine Cyanurate**	**Melamine Polyphosphate**	**N-alkoxy Hindered Amine Reaction Products**
>9	>10[a]	9.8[a]	No data	<0[a]	<-2[a]	>10
Phosphonate Oligomer	**Polyphosphonate**	**Poly[phosphonate-co-carbonate]**	**Red Phosphorous**	**Resorcinol bis-diphenylphosphate**	**Substituted Amine Phosphate Mixture**	**TBBPA glycidyl ether, TBBPA polymer**
>7.2 [a]	>7.2 [a]	No data	No data	4.93	<-2[a]	No data
TBBPA bis (2,3-dibromo-propyl ether)	**Triphenyl Phosphate**	**Tris (tribromoneo-pentyl) Phosphate**	**Tris (tribromo-phenoxy)Triazine**	**Zinc Borate**		
>10[a]	4.59	No data	No data	No data		

[a] Estimated data.

Bioaccumulation Potential						
Relevance to exposure: Indicates the degree to which a chemical substance may increase in concentration within a trophic level. Bioconcentration describes the increase in concentration relative to the organism's surroundings (environmental sources); bioaccumulation generally includes dietary and environmental sources. As chemicals bioconcentrate or bioaccumulate, there is a higher potential for them to reach a level where a toxic effect may be expressed. Estimated and/or measured bioconcentration and bioaccumulation values are presented as ranges based on relevant DfE hazard categories for each chemical. The DfE criteria for bioaccumulation designations are assigned by the bioaccumulation factor (BAF) or log BAF. The designations for bioaccumulation potential are as follows: Very High (VH) if the BAF (log BAF) is > 5,000 (>3.7); High (H) if the BAF is between 5,000 (3.7-3) and 1,000; Moderate (M) if the BAF is between <1,000 and 100 (<3-2); and Low (L) if the BAF is < 100 (<2) (U.S. EPA 2011b).						
Decabromodiphenyl Ether	**Aluminum Diethyl phosphinate**	**Aluminum Hydroxide**	**Ammonium Polyphosphate**	**Antimony Trioxide**	**Bis (hexachlorocyclopentadieno) Cyclooctane**	**Bisphenol A bis-(diphenylphosphate)**
High (1,000-5,000)[b]	Low (<100)[a]	Low (<100)[a]	Low (<100)[a]	Low (<100)[a]	High (1,000-5,000)[b]	High (1,000-5,000)[b]
Brominated Epoxy Resin End-Capped with Tribromophenol	**Brominated Polyacrylate**	**Brominated Polystyrene**	**Confidential Brominated Epoxy Polymer #1**	**Confidential Brominated Epoxy Polymer #2**	**Confidential Brominated Epoxy Polymer Mixture #1**	**Confidential Brominated Epoxy Polymer Mixture #2**
Low (<100)[b]	Low (<100)[c]	Low (<100)[c]	Low (<100)[c]	Low (<100)[c]	Low (<100)[c]	Low (<100)[c]
Confidential Brominated Polymer	**Decabromodiphenyl Ethane**	**Ethylene bis-tetrabromophthalimide**	**Magnesium Hydroxide**	**Melamine Cyanurate**	**Melamine Polyphosphate**	**N-alkoxy Hindered Amine Reaction Products**
Moderate (<1,000)[a]	High (1,000-5,000)[d]	High (1,000-5,000)[b]	Low (<100)[a]	Low (<100)[a]	Low (<100)[a]	High (1,000-5,000)[b]
Phosphonate Oligomer	**Polyphosphonate**	**Poly[phosphonate-co-carbonate]**	**Red Phosphorous**	**Resorcinol bis-diphenylphosphate**	**Substituted Amine Phosphate Mixture**	**TBBPA glycidyl ether, TBBPA polymer**
High (1,000-5,000)[b]	High (1,000-5,000)[b]	Low (<100)[c]	Low (<100)[a]	High (1,000-5,000)[b]	Low (<100) [b]	Low (<100)[c]
TBBPA bis (2,3-dibromo-propyl ether)	**Triphenyl Phosphate**	**Tris (tribromoneo-pentyl) Phosphate**	**Tris (tribromo-phenoxy)Triazine**	**Zinc Borate**		
High (1,000-5,000)[b]	Moderate (100-1,000)	Moderate (100-1,000)[b]	High (1,000-5,000) [b]	Low (<100)[b]		

[a] Based on professional judgment. [b] Based on estimated data. [c] Based on EPA Sustainable Futures polymer assessment guidance. [d] Based on monitoring data.

Persistence

Relevance to exposure: Indicates the length of time required for a chemical substance to be completely converted to small building blocks including water, carbon dioxide, and ammonia ("ultimate degradation"). Persistence is typically expressed as a 'half-life', which is the time for the amount of the substance to be reduced by one half. For a DfE chemical alternatives assessment, persistent chemicals include those that have metabolic or degradation products that have long half-lives. The longer a chemical or its degradation/metabolism products exist in the environment, the higher the likelihood for human or environmental exposure. "Compartments" refer to those environmental media to which chemicals may partition and include soil, sediment, water and air as standard compartments for fate assessment. Persistence is considered Very High (VH) if the half-life is > 180 days or recalcitrant; High (H) if the half-life is 60-180 days; Moderate (M) if the half-life is < 60 days but ≥ 16 days; Low (L) if half-life is <16 days OR readily passes biodegradability test not including the 10- day window (see Design for the Environment Program Alternatives Assessment Criteria for Hazard Evaluation); and Very Low (VL) if passes biodegradability test with 10-day window (see Design for the Environment Program Alternatives Assessment Criteria for Hazard Evaluation).

Decabromodiphenyl Ether	**Aluminum Diethyl phosphinate**	**Aluminum Hydroxide**	**Ammonium Polyphosphate**	**Antimony Trioxide**	**Bis (hexachlorocyclopentadieno) Cyclooctane**	**Bisphenol A bis-(diphenylphosphate)**
Very High (>180 days)	Very High (>180 days)[b]	High (60-180 days)[b]	Very High (>180 days)[c]	High (60-180 days)[b]	Very High (>180 days)	High (60-180 days)
Brominated Epoxy Resin End-Capped with Tribromophenol	**Brominated Polyacrylate**	**Brominated Polystyrene**	**Confidential Brominated Epoxy Polymer #1**	**Confidential Brominated Epoxy Polymer #2**	**Confidential Brominated Epoxy Polymer Mixture #1**	**Confidential Brominated Epoxy Polymer Mixture #2**
Very High (>180 days)[c]	Very High (>180 days)[c]	Very High (>180 days)[c]	Very High (>180 days)[c]	Very High (>180 days)[c]	Very High (>180 days)[c]	Very High (>180 days)[c]
Confidential Brominated Polymer	**Decabromodiphenyl Ethane**	**Ethylene bis-tetrabromophthalimide**	**Magnesium Hydroxide**	**Melamine Cyanurate**	**Melamine Polyphosphate**	**N-alkoxy Hindered Amine Reaction Products**
Very High (>180 days)[c]	Very High (>180 days)	Very High (>180 days)	High (60 – 180 days)[b]	Very High (>180 days)	High (60-180 days)[b]	High (60-180 days)
Phosphonate Oligomer	**Polyphosphonate**	**Poly[phosphonate-co-carbonate]**	**Red Phosphorous**	**Resorcinol bis-diphenylphosphate**	**Substituted Amine Phosphate Mixture**	**TBBPA glycidyl ether, TBBPA polymer**
Very High (>180 days)[a]	Very High (>180 days)[a]	Very High (>180 days)[a]	High (60-180 days)	Moderate (60 – 16 days)	High (60 – 180 days)[b]	Very High (>180 days)[c]
TBBPA bis (2,3-dibromo-propyl ether)	**Triphenyl Phosphate**	**Tris (tribromoneo-pentyl) Phosphate**	**Tris (tribromo-phenoxy)Triazine**	**Zinc Borate**		
Very High (>180 days)	Low (<16 days)	High (60-180 days)[a]	Very High (>180 days)	High (60-180 days)[b]		

[a] Based on results from biodegradation estimation model. [b] Based on professional judgment. [c] Based on EPA Sustainable Futures polymer assessment guidance.

5.2 Extraction

This section describes the first step in manufacturing a flame retardant, extracting or synthesizing the basic components which make up the final chemical. As stated in Chapter 3, there are four main categories of flame retardants: inorganic (i.e., metal salts), halogenated (bromine or chlorine), phosphorous-based, or nitrogen-based. Descriptions by category are given below demonstrating how the basic elements of each of the flame retardants for this assessment are extracted, and some exposure considerations associated with extraction are also included. This report is not evaluating the synthesis and processing of each of these materials but is providing information on the primary source of each of their components. In general, the organic flame retardants are derived from petroleum and the inorganic flame retardants are derived from other naturally occurring mineral deposits.

5.2.1 Inorganic Flame Retardants

The inorganic flame retardants considered in this report include the following base elements:

Aluminum

Aluminum, used in aluminum hydroxide ($Al(OH)_3$), is one of the most plentiful elements in the earth's crust and is usually present as bauxite ore. Bauxite can contain three different aluminum minerals, including gibbsite ($Al(OH)_3$), böhmite, and diaspore (crystalline structures of AlO(OH)). Bauxite ore also typically contains clay, silt, iron oxides, and iron hydroxides. The majority of bauxite is mined from surface deposits, but some is excavated from underground deposits (International Aluminium Institute 2007). Nearly all of the bauxite consumed in the United States is imported (USGS 2007). By refining bauxite ore using the Bayer process aluminum hydroxide can be made (U.S. EPA 1995b). This process requires mixing finely ground bauxite with sodium hydroxide to form a slurry that is then placed under steam pressure and heat (U.S. EPA 1995a). This creates a mixture of dissolved aluminum oxides and bauxite residues and precipitates out most of the impurities. The remaining slurry contains sodium aluminate that is flash cooled by evaporation and clarified to remove any other fine impurities (U.S. EPA 1995a). Lastly, the solution is sent to a precipitation tank where it is cooled and gibbsite "seeds" (usually from a previous cycle) are added to promote the precipitation of solid aluminum hydroxide crystals (U.S. EPA 1995a).

Magnesium

The mineral form of magnesium hydroxide ($Mg(OH)_2$), also called brucite, is found throughout the world (Amethyst Galleries Inc 2008; USGS 2008). However, magnesium hydroxide is typically recovered from seawater and magnesia-bearing brines, which constitutes an even greater and more readily available resource than brucite. In 2007, magnesium oxide and other magnesia compounds (including magnesium hydroxide) were recovered from both seawater and well brines in the U.S. (USGS 2008).

Antimony

Antimony (Sb), used in antimony trioxide (Sb_2O_3), can be mined, recovered as a byproduct from the smelting of lead and silver-copper ores, or derived from scrap source materials, including lead-acid batteries (Carlin Undated). Six U.S. companies produce antimony metal and oxide using domestic and foreign feed material (Carlin Undated). However, recycling and domestic mine output supplied less than half of the estimated U.S. demand for antimony, meaning a significant amount of antimony in the U.S. is imported (Carlin Undated). Antimony is mined as a principal product and recovered as a byproduct of the smelting of base metal ores in 23 countries. China, Bolivia, Russia and South Africa account for more than 90 percent of mine production (Carlin Undated). More than 50 percent of available antimony is used in flame retardants (Carlin Undated).

Zinc

Zinc most often occurs in association with the sulfide mineral group as sphalerite (ZnS), which is the principal mineral mined to recover zinc. Other metals associated with sulfide ores include copper, iron, mercury, cadmium, silver and small quantities of gold (U.S. EPA 1994b). These metals occur in varying amounts, and depend on the nature of the ore. Zinc ore is recovered from three types of deposits: strata-bound deposits, replacement deposits and vein deposits (U.S. EPA 1994). The largest and most productive deposits are associated with expansive, relatively flat lying sedimentary deposits. The strata-bound zinc ore in these deposits are restricted to well-defined stratigraphic units (a distinct layer of sedimentary or igneous rock), typically limestone, dolomite, or shale (U.S. EPA 1994). Replacement and vein type deposits make up a smaller portion of mined zinc. For the most part, zinc is mined in underground operations, although there are a few surface operations (U.S. EPA 1994).

5.2.2 Halogenated Flame Retardants

Bromine

Bromine is collected from salt brines in the United States and China, from the Dead Sea in Israel and Jordan, and from ocean water in Wales and Japan (Sjodin, Hagmar et al. 1999; Thuresson, Bergman et al. 2006; Bromine Science and Environmental Forum 2007; Qu, Bi et al. 2007). Bromine is typically isolated via a series of redox reactions involving chlorine, sulfur dioxide and acid (MIT 2003; The University of York 2004). During these reactions the brine or seawater is acidified and then chlorinated to oxidize bromide to elemental bromine. At this stage, the bromine is volatilized from the seawater, but it is not concentrated enough for collection or liquefying, so sulfur dioxide is added to reduce the bromine to hydrobromic acid. Chlorine is then added to re-oxidize hydrobromic acid to bromine gas (Br_2). At this point, bromine gas is collected and condensed (Grebe, Bauman et al. 1942). While caustic substances are involved in these processes, they are typically contained in an enclosed tower to prevent worker exposure and environmental release.

Chlorine

Chlorine, one of the most abundant elements on earth (Kostick 2001), is found primarily as the chloride ion (Cl^-), which is a component of salt found deposited in the earth or dissolved in the oceans. Chlorine is produced industrially via the chloralkali process, which involves the electrolysis of an aqueous sodium chloride (a brine) through an ion exchanging membrane (ERG 2006). Chloride ions are oxidized at an anode on the membrane into chloride. In addition to chlorine, this chloralkali process yields hydrogen gas (H_2) and sodium hydroxide (NaOH). The chloralkali process accounts for more than 95 percent of global chlorine production (ERG 2006).

5.2.3 Phosphorous-Based Flame Retardants

Phosphorus-based flame retardants are commonly synthesized from phosphate rock, which contains the mineral apatite (an impure tri-calcium phosphate). Phosphate esters can also be derived from yellow phosphorus. Large deposits of phosphate rock are found in Russia, Morocco, Florida, Tennessee, Utah, and Idaho (Lide 1993/94). Tri-calcium phosphate, the essential ingredient of phosphate rock, is heated in the presence of carbon and silica in an electric furnace or fuel-fired furnace. Elementary phosphorus is liberated as vapor and may be collected underwater (Lide 1993/1994). While elementary phosphorus can form a diatomic molecule with a triple bond, it more readily forms a tetrahedral P_4 molecule. At room temperature, phosphorus can exist in an amorphous or semi-crystalline state, called red phosphorus, which is produced from white phosphorus by extended heating in an inert atmosphere (Calvert 2004).

As for yellow phosphorous, approximately 80 percent of the global phosphorus is mined in China in the form of phosphate ore (Shigeru 2007). Extracting yellow phosphorus from phosphate ore also involves the co-extraction of arsenic, mercury, lead and other heavy metals as impurities that should be well controlled and treated before disposal of wastewater. If producers of yellow phosphorus appropriately treat their wastewater, then environmental releases and human exposures can be prevented. However, improperly treated wastewater can lead to major adverse environmental impacts (Shigeru 2007).

Predictions suggest that the world may be approaching peak phosphorous, or the point in time when the maximum production rate is reached. Phosphate-rich rocks are becoming harder to find and the demand for rock phosphate will soon exceed supply (Ulrich, Malley et al. 2009; Beardsley 2011). Depending on the calculation, predictions of peak phosphorous are broad (between twenty and several hundred years away), with some researchers predicting that peak extraction could occur as early as 2030 (Ulrich, Malley et al. 2009). This could have serious economic consequences in that it could raise the cost of products which use phosphorous(Ulrich, Malley et al. 2009) such as fertilizer or phosphorous-based flame retardants. It is suggested that there are ways to manage and mitigate peak phosphorous given that there is “an abundant but often ignored source of phosphorous” in human and animal waste (Beardsley 2011)but technology to extract and use phosphorous from these sources is still in its infancy (Ulrich, Malley et al. 2009).

5.2.4 Nitrogen-Based Flame Retardants

Nitrogen is the largest constituent of the earth's atmosphere and is also present in all living organisms, proteins, and nucleic acids (Kramer 2000). Anhydrous ammonia is produced commercially through the Haber-Bosch process, in which nitrogen and hydrogen react under high temperatures and pressure to produce ammonia (Kramer 2000). In this reaction, the source of nitrogen is air, which is almost 80 percent nitrogen. Additionally, small quantities of nitrates are mined from mineral resources principally in Bolivia and Chile (Kramer 2000). Although the U.S. produces most of its ammonia, the U.S. does import some ammonia mainly from Canada, Russia, and Trinidad and Tobago.

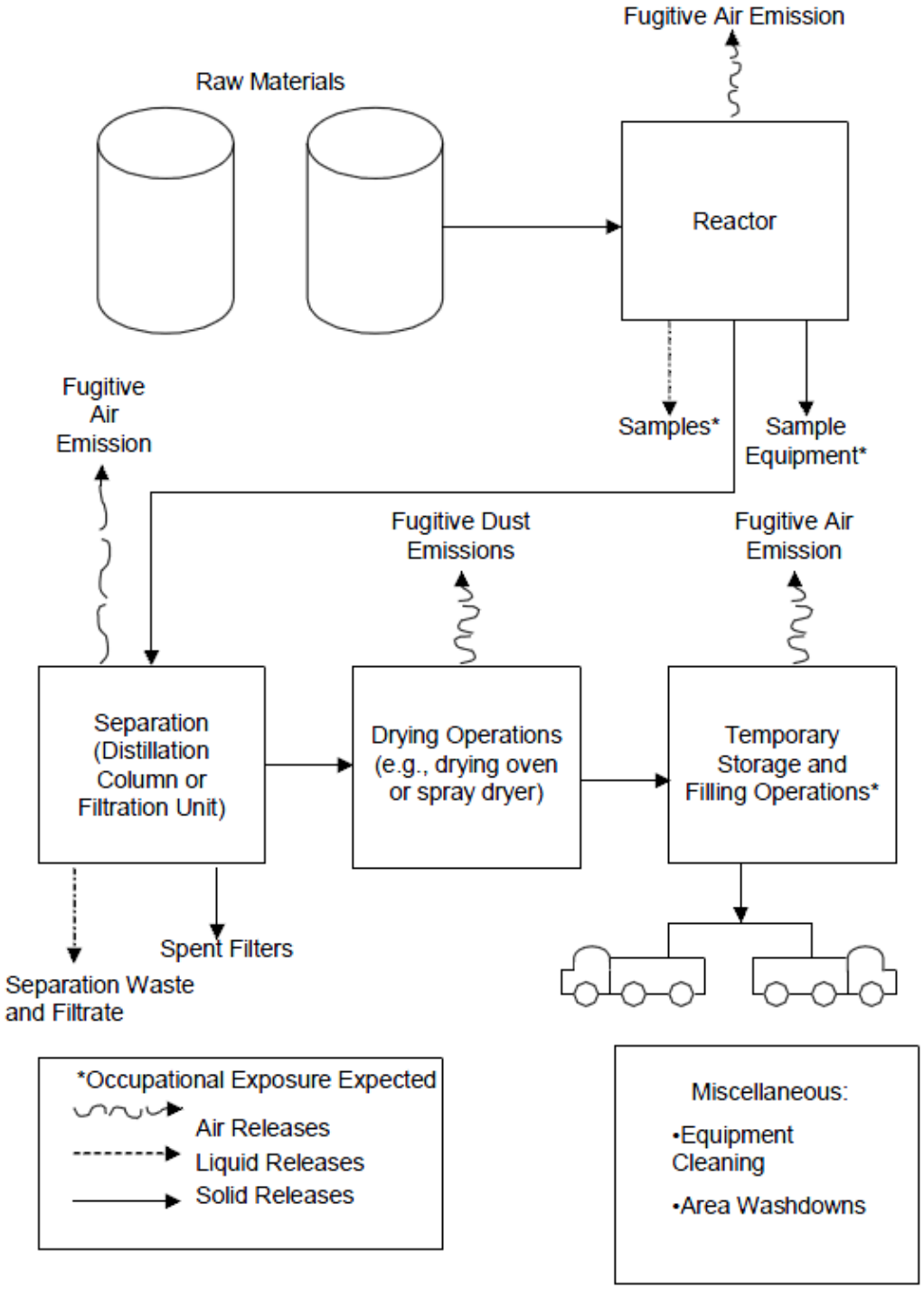
5.3 Chemical Manufacturing

After the extraction or synthesis of the flame retardant's basic components, the flame retardant chemical itself can be manufactured. Unit operations, operating conditions, transfer procedures, and packaging operations vary with the manufacture of different flame retardants and resin chemicals. Potential releases and occupational exposures will depend on each of these parameters. While it is outside the scope of this report to identify and quantify the releases and exposures associated with individual chemicals, this section presents a general description of typical chemical manufacturing processes and identifies potential releases.

Figure 5-2 is a generic process flow diagram for chemical manufacturing. Production volumes and batch sizes associated with flame retardants typically require the raw materials to be stored in large tanks or drums until use. The first step in most chemical manufacturing processes is to load or charge raw materials into some type of reactor or mix tank. Production volumes and batch sizes associated with flame retardant chemicals typically require the raw materials to be stored in large tanks or drums until use. Large-quantity liquids are typically pumped into the reactor, and solids are weighed and transferred via conveyorized, mechanical systems. Small-quantity raw materials may be manually introduced or carefully metered via automated systems. Releases and exposures that are expected from these operations are associated with the raw materials, not the finished flame retardant product (U.S. EPA 2005a).

Throughout the chemical manufacturing process, there are several release points that may pose an opportunity for exposures to workers (see Figure 5-2) including packaging operations, leaks from pumps and tanks, fugitive emissions from equipment, cleaning of process equipment, and product sampling activities. Additionally, crude or finished products are often stored on-site in drums, day-tanks, or more permanent storage vessels until the chemical is packaged and shipped to the next user. The transfer and packaging operations, waste management activities, as well as any routine and unplanned maintenance activities, and spills or accidents may result in releases and exposures.

Figure 5-2: Generic Chemical Manufacturing Process Flow Diagram



Source: U.S. EPA 2005a

Crude or intermediate products may be transferred through a series of reactors, distillation columns, filtration systems, drying ovens, spray dryers, and other unit operations. These processes typically occur in closed systems, with engineering controls that serve both to regulate operating parameters such as temperature and pressure as well as to minimize fugitive releases. However, there is potential for a variety of solid and liquid releases from these operations, from cleaning process equipment and from sampling activity. Additionally, crude or finished products may be stored on-site in drums, day-tanks, or more permanent storage vessels until the flame retardant formulation is packaged and shipped to customers (e.g., foam and textile manufacturers). The transfer and packaging operations, including storage, are expected to result in releases of the flame retardant chemicals. Finally, miscellaneous operations, such as routine and unplanned maintenance or waste management activities, can result in considerable releases and exposures (U.S. EPA 2005a).

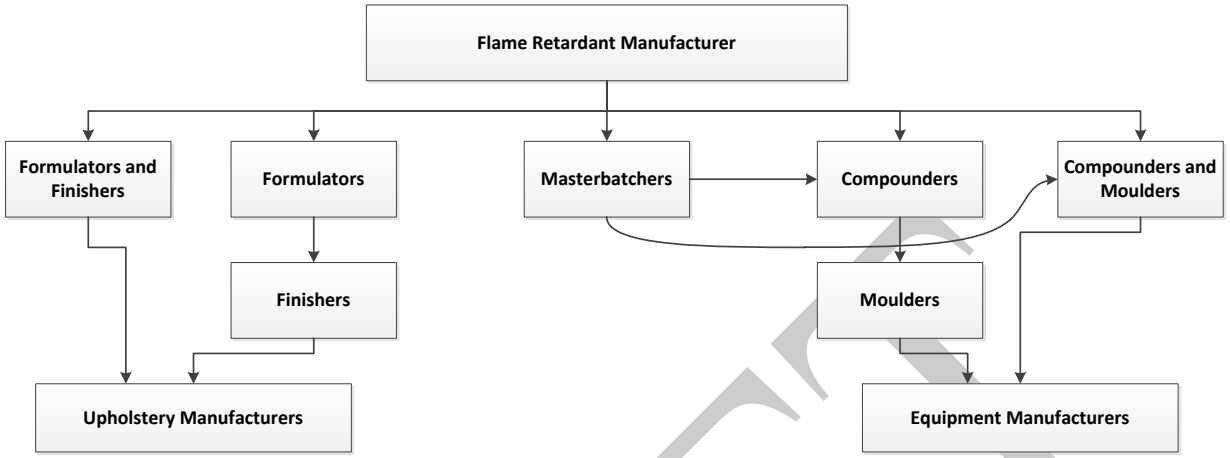
After the flame retardant is manufactured, it may need to be formulated into a solution, slurry, or mixture prior to its introduction into the commercial flame retardant formulation. For example, fine powders of a chemical may be formulated into an agglomerated powder or into a solution. The formulation steps usually occur at the chemical manufacturing facility, but additional mixing steps can occur at the formulator's manufacturing plant.

Release points from manufacturing and formulating can include: transfer and packaging operations involving handling a chemical product; routine and unplanned maintenance activities; leaks from pumps and pipelines; fugitive emissions from equipment; product sampling; waste management; and cleaning of equipment for transport and storage vessels.

5.4 Product Manufacturing

Given that decaBDE and its alternatives are used in a wide variety of products (see Chapter 2), this assessment does not include a discussion of the manufacturing process for each end-use product. However, a general discussion of how flame retardants are incorporated into plastics and textiles is included below in an attempt to understand where along the manufacturing process human or environmental exposures may occur. The production of flame retardants and their incorporation into a product is a complex process which involves multiple companies and specialties (European Chemicals Bureau 2002). With this in mind, the description of product manufacturing provided in this report is a generic one that understands that exposure is likely to vary at different facilities. Figure 5-3 displays the various steps flame retardants go through before they are incorporated into a final product for sale. The left side of the figure depicts the textile manufacturing process whereas the right side of the figure depicts the plastic manufacturing process (the plastic is subsequently used to make equipment such as televisions or computers).

Figure 5-3: Schematic of Flame Retardant Production and Incorporation into End Product Process



Source: European Chemicals Bureau 2002

Depending on the processes and equipment used, exposure can occur at each stage of the manufacturing process. For non-textile based polymers (the right half of Figure 5-3) exposure can occur anywhere along the process such as during compounding[13] or masterbatch[14] production and these processes may or may not be carried out in the same facility. The type of polymer being manufactured does not affect release volumes; release is dependent on the type of system used (i.e., closed or open) and the amount of flame retardant used (European Chemicals Bureau 2002).

Exposure potential is highest during the handling of the raw flame retardant (European Chemicals Bureau 2002). For decaBDE, any losses during this stage will be to the air but it is expected that the dust will rapidly settle within the facility. Therefore, exposure may occur dermally or through inhalation. To understand the fate and potential exposure routes of the other alternatives, an understanding of their physical-chemical properties is essential (see Table 5-1). Additionally, compounding is prone to dust generation but losses are thought to be lower than the handling of the flame retardant itself. It is possible that losses may occur early in the mixing cycle and that localized containment may be used to recover the material (European Chemicals Bureau 2002). There may be releases to the air and to the atmosphere at this stage of the manufacturing process.

Textile manufacturing (the left half of Figure 5-3) is a complex process which involves fiber preparation, spinning, knitting, weaving, and dyeing among many other steps, all of which occur in the finishing or upholstery manufacturing steps. The addition of additive flame retardants in textiles occurs in the final stage of wet processing, which occurs before the product is cut and sewn. According to the International Agency for Research on Cancer (IARC), "textile workers are exposed to textile related dusts through the manufacturing process. During the spinning, weaving and knitting operations, exposure to chemicals is generally limited." During the

[13] Blending of the polymer with various additives
[14] Plastic compounds that contain high concentrations of additives which are subsequently mixed in the main polymer matrix.

finishing processes when flame retardant chemicals are applied, IARC states that workers typically have exposures to multiple chemicals, including crease-resistance agents, antimicrobial agents, and flame retardants (IARC 1990).

When incorporating flame retardants into textiles, surface treatment is often used. There are two types of surface treatments: finishes and coatings. Finishes are applied by impregnating the fabrics in an aqueous solution of the chemical. Coatings are applied by incorporating a layer of flame retardant to the fabric, generating a heterogeneous fabric/polymer composite. Flame retardants used for finishes include phosphates and polyphosphates, phosphorous amides, phosphonium derivatives, antimony trioxide, borax and boric acid or halogenated flame retardants. Flame retardants used for coatings include phosphates, phosphonates, and brominated derivatives, which may be applied as backcoatings in the form of a paste or foam (GnoSys UK LtD for the Department of Environment Food and Rural Affairs 2010). As of 2008, the leading flame retardant in backcoating on a wide range of fabrics including synthetic blends, is decaBDE, used with antimony oxide. New chemicals in development for textile coatings are polymers and copolymers of pentabromobenzyl acrylate (CAS Number: 59447-55-1). Additionally, insoluble ammonium phosphates have also been found to work well on charrable fabrics (Weil and Levchik 2008).

Flame retardants in textiles are classified according to their "laundry durability." A non-durable flame retardant is washed off immediately when soaked in water, but may resist dry cleaning. Semi-durable flame retardants resist water soaking and possibly a few washes, while durable flame retardants resist 50 to 100 washes (Weil and Levchik 2008). Washing of flame retarded fabric could result in releases to waste water treatment plants and eventually to the environment.

Flame retardants based mostly on phosphate or phosphonate salts are typically used on infrequently washed or disposable goods given that they are non- or semi-durable. In regards to durable finishes, tetrakis(hydroxymethyl)phosphonium salts reacted with urea and cured with gaseous ammonia have been used for about 50 years in cellulosic fabrics. Other competitive wash-durable phosphorus-based finishes are also in development. Furthermore, polyesters are flame retarded with phosphonate or hexabromocyclodecane in a "thermosol[15]" process (Weil and Levchik 2008).

5.5 Use

As discussed in Chapter 2, decaBDE and its alternatives are used in a wide variety of polymers and products, allowing for potential release into a home, office or vehicle. Given that all of the flame retardants in this assessment are additive (as opposed to reacted into the polymer matrix), the potential for the flame retardant chemical to migrate or be released from a product is present. As discussed in Section 3.1.1, additive flame retardants are incorporated into the product through physical mixing and are not chemically reacted into the polymer. Empirical data on decaBDE and other PBDEs in house dust demonstrate that additive flame retardants are being released

[15] The thermosol process is the process of incorporating flame retardants into synthetic fibers. To run this process, liquid flame retardants are dissolved or dispersed in water (emulsion). Freshly spun hot fiber passes through this solution and the flame retardant penetrates the surface of the fiber because its affinity to the polymer is higher than to water. When the fiber cools down the flame retardant stays close to the surface.

from products into the surrounding environment (Stapleton, Dodder et al. 2004). However, it is difficult to identify or quantify the primary sources of the additive flame retardants, given consumer products are not labeled or identified by specific treatments with flame retardant additives.

There are peer reviewed studies about PBDE and decaBDE exposures. For example, Trudel, Scherinder et al. (2011) found that the body burden[16] of PBDE mixtures is generally higher in the United States and Canada than in other countries, likely due to the more stringent fire safety performance standards in North America and the greater number of consumer products containing these flame retardants. Again using PBDEs as an example, it has been shown that in the U.S., a primary exposure pathway for PBDEs among consumers is inhalation or ingestion of house dust (Johnson, Stapleton et al. 2010). In contrast, the diet constitutes a primary exposure pathway for consumers in Europe, China, and many other countries worldwide (Trudel, Scheringer et al. 2011). PBDE's have a tendency to bioaccumulate in the food chain, particularly in fatty tissues of animals. Consequently, meat and dairy products have higher concentrations of PBDEs than fruit and vegetables (Schecter, Haffner et al. 2010). Additionally, a large number of human samples have been analyzed and PBDE concentrations have increased by nearly a factor of 100 during the last 30 years (U.S. EPA 2009a). The bioaccumulation potential of the other alternatives in this assessment is addressed in the Chapter 4 in each chemical's hazard evaluation.

Exposure levels and routes also vary by age group. Given children's predisposition to put hands and toys in their mouth, they can inadvertently ingest larger amounts of house dust than adults. Some children may be at a higher risk of exposure if family members work with PBDEs and bring dust containing the chemical home with them (Washington State Department of Labor & Industries Undated). The Agency for Toxic Substances and Disease Registry (ATSDR) (2004) and the Child-Specific Exposure Factors Handbook (2008a) both state that a child's exposure may differ from that of adults because children drink more fluids, eat more food, breathe more air per kilogram of body weight, and have a larger skin surface area in proportion to body volume. Additionally, it is possible for infants to be exposed to bioaccumulative chemicals through breast milk.

In addition to considering consumer exposures to a specific flame retardant, it is important to consider degradation products. For example, under certain conditions, decaBDE can degrade to less brominated congeners, which are potentially more toxic. Photolysis is expected to be the primary degradation process for decaBDE when it is significantly exposed to UV light (U.S. EPA 2009a). DecaBDE can undergo photolytic debromination in house dust (Stapleton and Dodder 2008) and in organic films exposed to sunlight through automobile windshields (Ecology Center 2008), demonstrating that debromination may be possible within an automobile. Metabolic debromination of decaBDE can occur in fish, birds, cows, and rats, although its overall significance when compared with other degradation processes is unclear (U.S. EPA 2009a). Uncertainty exists for the degradation products of some decaBDE alternatives. Debromination and other degradation processes may be relevant for some of the alternatives. Chapter 4 of this report provides a summary of the chemical-specific information available at the time of publication.

[16] Body burden refers to the amount of a toxic substance present in the human body at a given time.

5.6 End-of-Life

When products reach their end-of-life, there are multiple pathways which they could take, including recycling (including reuse and refurbishment), landfilling, or incineration. The manner in which a product is handled after use contributes to its environmental and human health impacts. The following sections consider end-of-life issues for some of the types of products requiring flame retardants. Note that there may be overlap in the information presented for each product sector.

5.6.1 Electronics

The amount of used and end-of-life electronic equipment generated annually in the United States is growing rapidly. In 2010, the U.S. electronics recycling industry processed over 3.5 million tons of used and end-of-life electronic equipment (a large increase compared to the 650,000 tons processed in 2002) (Institute of Scrap Recycling Industries Inc 2011), whereas 3.2 million tons, predominately from households, is still sent to landfills (U.S. EPA 2010e). However, the amount being sent to landfills is likely to decline as there is a growing trend of state laws that requires the recycling of used and end-of-life electronics equipment (U.S. EPA 2010e).

Recycling Electronics

The U.S. electronics recycling industry has grown over the past ten years and has the capacity to handle additional tonnage. The biggest challenge is the need to educate households, businesses and government entities on the importance of responsibly recycling their used electronics equipment (Harris 2011; Institute of Scrap Recycling Industries Inc 2011).

The U.S. electronics recycling industry has seen a significant increase in the use of third-party certifications for electronic waste management and recycling (Harris 2011; Institute of Scrap Recycling Industries Inc 2011). Electronics recyclers may be certified to the *Responsible Recycling Practices for Use in Accredited Certification Programs for Electronics Recyclers* – better known as the "R2 Practices", (or simply "R2") or the *e-Stewards Standard for Responsible Recycling and Reuse of Electronic Equipment*®, (as known as "the e-Stewards Standard").[17]. The e-Stewards Standard is another certification program by which electronics recyclers may be certified. The certification process helps to ensure that electronics recyclers use the best available practices to protect worker health by minimizing exposure.

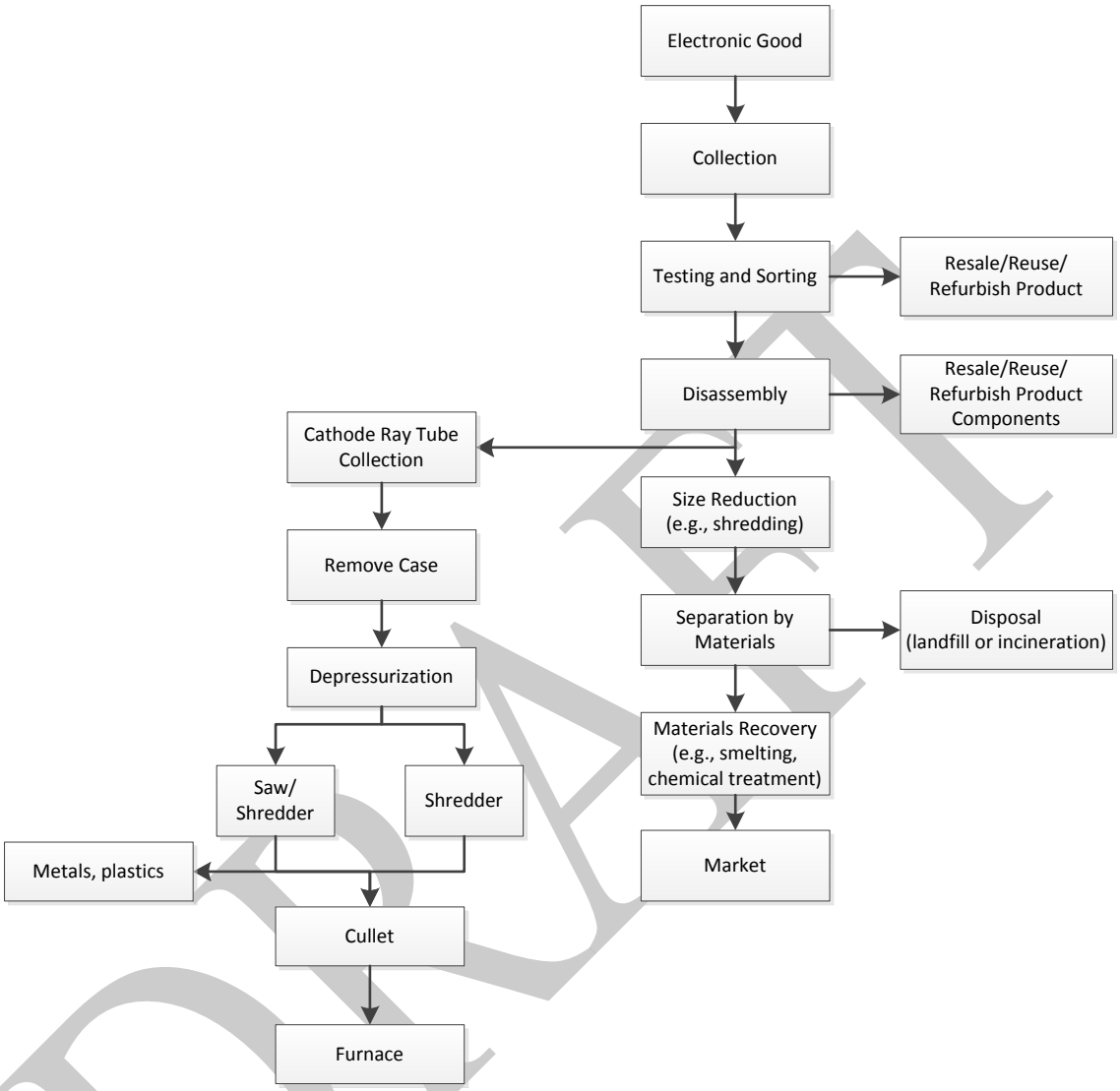
In the United States, used and end-of-life electronic equipment is typically collected by the recycling industry (i.e., collectors, repair/refurbishers, recyclers, and brokers). The collected equipment then undergoes a series of tests, or is "triaged", to determine its condition and market value, if any. If a device or component's key functions are in good working condition it can be resold directly as a used product or refurbished (e.g., updated operating systems or cosmetic changes) and then sold as a product on the domestic and global marketplace.

[17] Information about electronics recycling facilities certified to the R2 Practices is available from R2 Solutions at www.R2Solutions.org. For more information about electronics recycling facilities certified to the e-Stewards Standard, go to www.estewards.org.

After the triage process, the remaining equipment is disassembled, either manually or mechanically, and segregated into commodity grade streams (e.g., steel, aluminum, plastic, glass, circuit boards that include copper, gold, silver, platinum, palladium, and rare earth oxides) that are then sold into the domestic and international commodities market. Many of the markets for processed raw materials are also outside of the U.S. and the manner in which used electronics are disposed of or recycled will affect the potential environmental and human health impacts.

Figure 5-4 is a depiction of the general electronic recycling process and shows that this process can involve both thermal processing, such as smelting to recover precious metals, and nonthermal processing, such as disassembly, shredding, separation, and chemical treatment (Kang and Schoenung 2005). The potential level of exposure to workers and the general population that results from these processes will vary depending on the management practices used within a facility.

Figure 5-4: Electronics Recycling Process



Source: Adapted from Kang and Schoenung 2005

The potential for emissions of halogenated dioxins and furans, mercury, lead, antimony, and other toxic substances exists with smelting operations that may be a part of the recycling process. In addition to the potential emission of toxic chemicals, high operating temperatures may create an occupational hazard and high loads of bromine or chlorine may induce corrosion of gas-cleaning equipment. In sensitive areas, a process step for halogenide recovery may need to be added (Lehrner 2008). Controlled smelting operations are able to handle high loads of halogenated electronic scrap and effectively control emissions.

Some post-use electronics are exported for reuse, refurbishment and recycling. Unfortunately, a number of these exported electronics end up in countries that do not have the technology to

recycle the electronics in a way that does not pose exposure concerns.. In the absence of proper practices, procedures and equipment, unregulated recycling processes may pose risks to workers and the public through exposure to toxic chemicals.

Additionally, a 2007 U.S. EPA study examined the waste management of computer, television, hard-copy devices, and cellular devices. The study indicated that 15 to 20 percent of post-use consumer electronics was recycled, and 80 to 85 percent was disposed of in landfills or through incineration (U.S. EPA 2007b).

The methods employed at these unregulated recycling sites are sometimes crude and may include the open burning of printed circuit boards, cables, and plastics; acid or cyanide leaching of circuit boards; and gold recovery with cyanide salt leaching or nitric acid and mercury amalgamation (Williams, Kahhat et al. 2008; Sepúlveda, Schluep et al. 2010; Yu, Williams et al. 2010). These methods may pose concern for human and environmental health. Toxic substances released from these processes include leachates, particulate matter, fly and bottom ash, fumes, wastewater, and other effluents, which are released to the soil, groundwater, surface water, sediments, and air (Sepúlveda, Schluep et al. 2010). For example, the burning of electronic components containing flame retardants can produce a range of toxic by-products including halogenated dioxins and furans (U.S. EPA 1998; Tohka and Zevenhoven 2002).

Landfilling Electronics

More than 3.2 million tons of end-of-life electronics, predominately from households, are sent to landfills (U.S. EPA 2010e). Landfills in the United States are for the most part well managed and regulated, but in non-regulated and non-lined landfills, these post-use electronics can contribute to leachate (i.e., the mixture of rainwater and liquids within the waste). This leachate has the potential to seep into the ground or drain into nearby surface water, transporting chemicals where humans and wildlife may be exposed. Additive flame retardants have a higher potential than reactive flame retardants to be released from electronic products (KemI 1995). No reactive flame retardants were identified as alternatives to decaBDE.

To date, most leachability studies in the literature have focused on the potential for discarded electronic devices to release lead and other heavy metals. A small number of studies have investigated leaching potential of brominated flame retardants. For example, Osako et al, (2004) found that the levels of several PBDEs congeners in both raw and treated leachate were below the limit of detection of 4,000 pg/L (Osako, Kim et al. 2004). Additionally, a study conducted by Beard and Marzi (2006) investigated the leachability potential of phosphorus-based and brominated flame retardants from thermoplastic polymers and found that small amounts of phosphorus and bromine, respectively, leached from the polymer (Beard and Marzi 2006). Osako et al. (2004) also concluded that the amount of leaching that occurs is dependent upon the chemical properties of the landfill (Osako, Kim et al. 2004).

Incineration of Electronics

According to EFRA, flame retarded plastics can be incinerated in municipal refuse incinerators as long as they are equipped with the proper gas cleaning devices (EFRA 2006). The flame retardant treatment will not prevent incineration at operating temperature.

EPA has done an alternatives assessment for flame retardants used in printed circuit boards, the final report of which will include data on combustion by-products for different burning scenarios. The final report will be posted to the DfE webpage: http://epa.gov/dfe/pubs/projects/pcb/index.htm

5.6.2 Textiles

DecaBDE and its alternatives are often used in the textiles which make up office furniture, commercial grade carpet, or military supplies such as tents, tarps and uniforms. Below is a summary of information on the various textiles, specifically office furniture and commercial grade carpet, which may enter each end-of-life pathway.

Recycling Textiles

Only ten percent of the six billion pounds of carpet disposed of in 2010 was recycled, reconditioned, or reused (Carpet America Recovery Effort (CARE) 2010). As a response to the high rate of carpet disposal in landfills, members of the carpet industry, representatives of government agencies at the federal, state, and local levels (such as the U.S. EPA), and non-governmental organizations created a voluntary partnership in 2002 to increase the amount of post-consumer carpet reused, reconditioned, or recycled. The goal of the ten-year partnership is to reduce the amount of carpet discarded in landfills by 40 percent by 2012 by diverting the carpet to one of four routes: reuse, recycling, waste to energy (incineration technology that uses recovered carpet as a fuel source to generate electricity), or cement kilns (the use of a recovered carpet as an alternative fuel source and as an additive in cement production) (CARE 2006). In order to achieve this benchmark, the carpet industry created the CARE, which, with members of the carpet industry and government, is responsible for monitoring, evaluating, and assessing progress toward the negotiated goals (CARE 2006).

Landfilling Textiles

The frequent replacement of office furniture results in the increased production of products and leads to large volumes of furniture discarded in landfills. Landfilling is also the most common fate of used carpeting. Even though almost all of the components in carpet can be recycled or reused, the total estimated amount of U.S. carpet discarded in 2010 was six billion pounds (CARE 2010).

Research with the objective of investigating the release and transformation of additive and reactive flame retardants from textiles in simulated landfill environments was conducted in 2008 (Horsing 2008). The study found that the environmental conditions of a landfill (e.g., temperature, microbial activity, and pH), the way additives are applied (i.e., additive or reactive), and the nature of the material all affected the leaching of the flame retardants. Based on the findings of the impact of the different landfill conditions on additive flame retardants, the author concluded that additive flame retardants may "leach and contribute to the contamination of water but not so much in new, well-managed landfills and in developed countries as in old landfills in countries where landfills are poorly managed" (Horsing 2008). Additionally, they found that the

only leaching that occurred from products treated with reactive flame retardants was washout from unreacted manufacturing residuals.

Incineration of Textiles

Incineration of textile waste from production sites is difficult given that pieces of fabrics are too long and can cause fire outside the incinerator. The textiles are usually too strong to be ground prior to incineration. Therefore large amounts of textile waste from textile plants are landfilled instead of incinerated (Dahllof 2004). However, smaller flame-retarded textiles and foams can be incinerated. This method is preferred as long as the incinerators are equipped with the proper gas cleaning devices (EFRA 2006).

5.6.3 Storage and Distribution Products

A total of two to three billion storage and distribution pallets, composed of a variety of components including wood, plastic, aluminum, steel, corrugated paperboard, and composite wood, are believed to be in use in the United States (Buehlmann, Bumgardner et al. 2009; Pure Strategies Inc. for Maine Department of Environmental Protection 2010). Wood currently dominates the pallet market and is estimated to comprise 80 to 95 percent of pallets (Buehlmann, Bumgardner et al. 2009; Pure Strategies Inc. for Maine Department of Environmental Protection 2010). Wood's overwhelming presence in the pallet market is due to its low material and production costs and its relative abundance as a raw material. However, the use of plastic pallets is becoming increasingly popular because plastic often is more durable, lighter, and more easily sanitized than wood. In 2010, over 900 million plastic pallets were estimated to be in use (Pure Strategies Inc. for Maine Department of Environmental Protection 2010).

Depending on the materials and construction, and the manner in which they are used, plastic pallets could have an expected lifetime of 20 years. Many plastic pallets are made from recycled plastic and are fully recyclable at the end of their lives (Pure Strategies Inc. for Maine Department of Environmental Protection 2010). When plastic pallets are no longer usable, they are removed from service and can enter a full recycling process (ERM 2008). One manufacturer of high-density polyethylene (HDPE) pallets shreds or grinds damaged pallets for reuse as a raw material, which, in turn, is molded into new pallets. Currently, new plastic pallets are sometimes made with a combination of recycled and new HDPE but the recycled content may increase in the long term. According to one producer of plastic pallets, small quantities of HDPE that might be trimmed or removed during fabrication, handling and processing of extruded plastic are collected for reuse at the pallet production facility.

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6 Considerations for Selecting Flame Retardants

Selecting an alternative chemical flame retardant involves considering a range of factors. DfE chemical alternatives assessments provide extensive information on chemical hazards and provide a more general discussion of other factors relevant to substitution decisions, such as: use information, exposure considerations and performance. Decision-makers will likely supplement the human health and environmental information provided in this report with information on cost and performance that may vary depending on the supplier, the materials involved, and the intended application. Alternative flame retardants must not only have a favorable environmental profile, but also must provide satisfactory (or superior) fire safety, have an acceptable cost, and attain the appropriate balance of properties (e.g., mechanical, thermal, aesthetic) in the final product. Users of information in this report may wish to contact the manufacturers of alternative flame retardants for engineering assistance in designing their products with the alternatives.

This chapter outlines attributes that are appropriate for a decision maker to consider in choosing an alternative to decaBDE. The chapter begins by describing five general attributes evaluated in this assessment that can inform decision-making about chemical hazards: (1) human health, (2) ecotoxicity, (3) persistence, (4) bioaccumulation potential and (5) exposure potential. The chapter gives special attention to discussion of data gaps in the full characterization of chemicals included in this assessment. The chapter includes information on the social, performance, and economic considerations that may affect substitution. The chapter concludes by providing additional resources related to state, federal, and international regulations.

The scope of this assessment was focused on the human health and environmental hazards of potential flame retardant substitutes. The report does not include a review or analysis of any additional life-cycle impacts, such as energy and water consumption or global warming potential, associated with any of the baseline or alternative chemicals, or the materials in which they are used. If selection of an alternative flame retardant requires significant material or process changes, relevant life cycle analyses can be applied to the viable alternatives identified through this hazard-based alternatives assessment, and to the materials in which they are used. Manufacturers may also wish to analyze the life-cycle impacts of materials that do not require the use of a flame retardant, in order to select materials that pose the fewest life-cycle impacts.

6.1 Preferable Human Health and Environmental Attributes

This section identifies a set of positive attributes for consideration when formulating or selecting a flame retardant that will meet flammability standards. In general, a safer chemical has lower human health hazard, lower ecotoxicity, better degradability, lower potential for bioaccumulation and lower exposure potential. As described in Chapter 4, the toxicity information available for each of the alternatives varies. Some hazard characterizations are based on measured data, ranging from one study to many detailed studies examining multiple endpoints, doses and routes of exposures. For other chemicals, there is no chemical-specific toxicity information available, and in these cases either structure activity relationship (SAR) or professional judgment must be used. In Table 4-4, Table 4-5and Table 4-6Appendix A the hazard designations based on SAR or professional judgment are listed in black italics, while those with hazard designations based on measured test data are listed in color. Readers are encouraged to review the detailed hazard assessments available for each chemical in Chapter 4.

6.1.1 Low Human Health Hazard

The DfE alternatives assessment criteria address a consistent and comprehensive list of human health hazard endpoints. Chemical hazards to human health include: acute toxicity, carcinogenicity, genotoxicity, reproductive and developmental toxicity, neurotoxicity, repeated dose toxicity, skin sensitization, respiratory sensitization, eye irritation and dermal irritation. The DfE criteria have thresholds established to define low, moderate, and high hazard. As described in Chapter 4, where data for certain endpoints were not available or were inadequate, hazard values were assigned using data for structural analogs, structure-activity relationship (SAR) modeling and professional judgment. In some cases (e.g., respiratory sensitization) it was not possible to assign hazard values due to a lack of data, models or structural analogs.

For the flame retardant chemicals evaluated in the report, human health hazard endpoints varied due to the different chemistries of decaBDE and the 32 alternatives. Some general trends include the following:

1. Large polymers (greater than 1,000 daltons) were generally designated as low concern compared to discrete chemicals, because the large polymers generally cannot be absorbed or easily metabolized. Chemicals with molecular weights close to 1,000 may have potential for absorption whereas those with molecular weights much larger than 1,000 have a much lower potential for absorption (U.S. EPA 2010d). Without absorption there cannot be systemic effects. Although irritation can occur without absorption, it was not identified as a hazard for any of the large polymers and therefore was not a distinguishing characteristic in this assessment.

2. Acute mammalian toxicity was low for decaBDE and all the alternatives, with two exceptions: red phosphorus and the substituted amine phosphate mixture.

3. Irritation and sensitization endpoints were generally not distinguishing, but seven chemicals had at least one designation of moderate, high, or very high for one or more irritation or sensitization endpoint, whereas decaBDE has low designations for these endpoints.

4. Carcinogenicity and mutagenicity hazards varied among the alternatives, with many low or moderate results. None of the chemicals had high concerns for carcinogenicity. Only zinc borate had a high concern for mutagenicity. DecaBDE was low for genotoxicity and moderate for carcinogenicity.

5. Reproductive, developmental, neurological, and repeated dose toxicity varied from low to high across discrete chemicals. DecaBDE has high developmental and neurological toxicity and moderate repeated dose toxicity.

6.1.2 Low Ecotoxicity

Ecotoxicity includes adverse effects observed in wildlife. Aquatic organisms have historically been the focus of environmental toxicity considerations by industry and government during

industrial chemical review. Surrogate species of fish, aquatic invertebrates and algae are traditionally assessed to consider multiple levels of the aquatic food chain. Aquatic organisms are a focus also because the majority of industrial chemicals are released to water. Both acute and chronic aquatic toxicity should be considered in choosing a chemical flame retardant. Where data or expert knowledge are available, ecotoxic effects on other classes of animals and plants should be included in the hazard evaluation; some human health data (i.e., exposures to rodents) can be relevant to non-human vertebrates in ecotoxicity evaluations. When evaluating potential concerns for higher trophic level organisms (including humans), bioaccumulation potential (discussed in Section 6.1.4) is an important consideration for choosing a safer alternative.

For the flame retardant chemicals evaluated in the report, ecotoxicity hazards varied significantly due to the diverse chemistries of the alternatives. Some general trends include the following:

1. Large discrete chemicals and large polymers (both halogenated and non-halogenated) had generally low ecotoxicity hazards. The larger chemicals and compounds with high K_{ow} values are not expected to be bioavailable in the water column. Without absorption there cannot be systemic effects. For almost all these chemicals (including decaBDE) the hazard designation was based on professional judgment and/or SAR predicting 'no effects at saturation'.

2. For inorganic compounds, aquatic toxicity varied from low to very high. The metal species influences toxicity, as does the type of anion with which it is associated (e.g., a metal hydroxide). Metal compounds will have different solubilities depending on the anion involved, which will contribute to the level of toxicity of the metal compound. The aluminum, antimony and zinc compounds have moderate to very high aquatic toxicity. For aluminum hydroxide, sufficient data are not available to rule out a moderate concern. For magnesium hydroxide and red phosphorus, aquatic toxicity was low based on predicted and measured data, respectively.

3. In addition to some of the inorganic compounds, some of the phosphorus and/or nitrogen-containing compounds also had high measured or predicted aquatic toxicity.

4. Ecotoxicity data for terrestrial species was limited or completely absent for the chemicals assessed.

6.1.3 Readily Degradable: Low Persistence

Persistence describes the tendency of a chemical to resist degradation and removal from environmental media, such as air, water, soil and sediment. Chemical flame retardants must be stable by design in order to maintain their flame retardant properties throughout the lifetime of the product. Therefore, it is not surprising that 31 of the 33 chemicals assessed in this report, including decaBDE, had a persistence value of high or very high. The alternatives without high concern for persistence were triphenyl phosphate, which is readily biodegradable (low persistence), as well as resorcinol bis-diphenyl phosphate (inherently biodegradable), which degrades slowly (moderate persistence). A number of the alternatives are high molecular weight polymers (>10,000 daltons) that are predicted to be highly persistent because they are not bioavailable or assimilated by microorganisms. Highly persistent chemicals may ultimately

degrade in the right environmental conditions, but time to degradation is much longer than other chemicals, often several months or years.

If the use of higher molecular weight chemicals and polymers for flame retardant applications increases, there would be a need for further information regarding the environmental fate of these chemicals to understand how they behave in the environment, including their persistence in various environmental settings and the identity and toxicity of their degradation products. Environmental monitoring information exists for some of the (non-polymeric) alternatives, including the degradation products, which have been in the marketplace for more than a few years. However, no information is available for other alternative chemicals.

Environmental monitoring could bolster hazard assessments by confirming that environmental fate is as predicted. The lack of such information should not be taken as evidence that environmental releases are not occurring. Environmental detection is not equivalent to environmental persistence; detection in remote areas (e.g., the Arctic) where a chemical is not manufactured is considered to be a sign of persistence and transport from the original point of release. An ideal safer chemical would be stable in the material to which it is added and have low toxicity, but also be degradable at end of life of that material, i.e., persistent in use but not after use. This quality is difficult to achieve for flame retardants.

The half-life for a given removal process is used to assign a persistence designation. The half-life measured or estimated to quantify persistence of organic chemicals is not a fixed quantity like the half-life of a radioisotope. Chemicals with half-lives that suggest low or no persistence can still present environmental problems. "Pseudo persistence" can occur when the rate of input (i.e., the emission rate) of a substance exceeds the rate of degradation in, or movement out of, a given area.

In addition to the rate of degradation or measured half-life, it is important to be aware of the byproducts formed through the degradation process. In some cases, degradation products might be more toxic, bioaccumulative or persistent than the parent compound. Some of these degradation products are discussed in the hazard profiles, but a complete analysis of this issue is beyond the scope of this assessment. Stakeholders are encouraged to conduct additional analyses of the degradation products of preferable alternatives using the assessment methods described in Chapter 4.

In general, metal-containing chemicals are highly or very highly persistent. This is because the metal moiety remains in the environment. Metal-containing compounds can be transformed in chemical reactions that could change their oxidation state, physical/chemical properties, or toxicity. A metal-containing compound may enter into the environment in a toxic (i.e., bioavailable) form, but degrade over time into its inert form. The converse may also occur. The chemistry of the compounds and the environmental conditions it encounters will determine its biotransformation over time. For metals, information relevant to environmental behavior is provided in each chemical assessment in Chapter 4 and should be considered when choosing an alternative.

6.1.4 Low Bioaccumulation Potential

The ability of a chemical to accumulate in living organisms is described by the bioconcentration, bioaccumulation, biomagnification, and/or trophic magnification factors. DecaBDE has high concern for bioaccumulation, as do its break down products (lower brominated diphenyl ether congeners). Some of the alternatives assessed in this report have a high level of potential for bioaccumulation, including the discrete brominated chemicals and, based on presence of oligomers below 1,000 daltons, the phenyl phosphates. Based on structure activity relationships, the potential for a molecule to be absorbed by an organism tends to be lower when the molecule is larger than 1,000 daltons. This is reflected in the low hazard designations for bioaccumulation for the polymeric flame retardants without low molecular weight components below 1,000 daltons. The inorganic flame retardants assessed in this report do not have high potential to bioaccumulate, nor do the discrete nitrogen based flame retardants. Note that care should be taken not to consider the 1,000 daltons size to be an absolute threshold for absorption – biological systems are dynamic and even relatively large chemicals might be absorbed under certain conditions. In the past, available data suggested that the large size of decaBDE would preclude transport across biological membranes and that its limited water solubility would decrease the potential for absorption (Toxicology Excellence for Risk Assessment 2003). Absorption of decaBDE is poor, whereas lower brominated polybrominated diphenyl ethers (PBDEs) are readily absorbed (ATSDR 2004). Subsequent studies using more sensitive analysis techniques have detected the substance in biological samples demonstrating its potential to be absorbed (Lorber 2008). DecaBDE has a molecular weight of 959 daltons. This provides a basis to suggest that the potential for absorption and potential for bioaccumulation of large molecules around 1,000 daltons is not well understood.

Chemical manufacturers have reduced absorption and bioaccumulation potential through the design of larger molecules. Making a molecule bigger (often by making large polymeric molecules) can reduce bioavailability, or minimize the likelihood of low molecular weight components and residuals of concern. A larger polymeric flame retardant molecule may also impact performance properties of the material to which the flame retardant is added in positive or negative ways. A safer molecule also has to perform well in the intended application.

The test guidelines available to predict potential for bioaccumulation have some limitations. Bioconcentration tests tend to be limited for chemicals that have low water solubility (hydrophobic), and many flame retardants have low water solubility. Even if performed properly, a bioconcentration test may not adequately measure bioaccumulation potential if dietary exposure dominates over respiratory exposure (i.e., uptake by fish via food versus via their gills). Under review in the Organisation for Economic Cooperation and Development program and close to finalization is a major upgrade to the fish bioconcentration test, in which dietary uptake is included for the first time (OECD 2012). Dietary uptake is of critical importance and may be a more significant route of exposure for hydrophobic chemicals.

6.1.5 Low Exposure Potential

For humans, chemical exposure may occur at different points throughout the chemical and product lifecycle; by dermal contact, by inhalation, and/or by ingestion; and is affected by multiple physicochemical factors that are discussed in Chapter 5. The DfE alternatives

assessment assumes exposure scenarios to chemicals and their alternatives within a functional use class are roughly equivalent. The assessment also recognizes that in some instances chemical properties, manufacturing processes, chemical behavior in particular applications, or use patterns may affect exposure scenarios. For example, some decaBDE flame retardant alternatives may require different loadings to achieve the same flammability protection. Stakeholders should evaluate carefully whether and to what extent manufacturing changes, lifecycle considerations, and physicochemical properties will result in different patterns of exposure as a result of informed chemical substitution. For example, a decaBDE replacement which is not soluble in the polymer it is flame retarding may leach out, or "bloom" out of the polymer faster, thus increasing exposure while the flame retardant polymer is in use or when it is disposed. The combination of high persistence and high potential for bioaccumulation makes an alternative less desirable. Even if human toxicity and ecotoxicity hazards are measured or estimated to be low, dynamic biological systems don't always behave as laboratory experiments might predict. High persistence, high bioaccumulation chemicals, or their degradation products, have high potential for exposure and unpredictable hazards following chronic exposures that may not be captured in the hazard screening process.

6.2 Considerations for poorly or incompletely characterized chemicals

Experimental data for hazard characterization of industrial chemicals are limited. As described in Chapter 4, for chemicals in this report without full data sets, analogs, SAR modeling, and professional judgment were used to estimate values for those endpoints lacking empirical data. No alternative chemical had empirical data for all of the hazard categories. Nine chemicals had no empirical data at all, and all of their respective endpoints were predicted; an additional six lacked data on at least 10 of the hazard endpoints. Several chemicals included in this analysis appear to have more preferable profiles, with low human health and ecotoxicity endpoints, although they are highly persistent, a frequent property for flame retardants (see Table 4-4, Table 4-5 and Table 4-6). However, because most of the hazard designations were based on estimated effect levels, there is less confidence in the results. Empirical data would allow for a more robust assessment that would confirm or refute professional judgments and then support a more informed choice among alternatives for a specific use. Estimated values in the report can, therefore, also be used to prioritize testing needs.

Examples where data are lacking for end points reviewed for chemicals in this report include the following:

1. The environmental fate of large discrete or polymeric flame retardants (molecular weight approaching or exceeding 1,000 daltons) is uncertain. This is true for both halogenated and nonhalogenated chemicals. Polymeric flame retardants are assessed in this report as functional alternatives to decaBDE. Some of these polymeric chemicals were designed to be safer alternatives to decaBDE. While SAR analysis shows these chemicals are anticipated to be associated with low hazard, chemical-specific data to support these predictions are lacking. In general, large polymeric flame retardants are predicted to have high persistence but low concern for toxicity or potential for bioaccumulation. Further research is needed to fully understand the environmental fate of polymers approaching or exceeding 1,000 daltons.

2. For discrete brominated chemicals with molecular weight and (or) functional groups similar to decaBDE, hazard designations were based on analogy to decaBDE. Because of reactivity, physicochemical and structural properties similar to those of decaBDE, chronic exposure studies are needed to rule out concerns similar to those that have been raised regarding long-term exposure to decaBDE.

3. Empirical data is needed to confirm low toxicity and bioaccumulation predictions. Flame retardants are usually highly persistent chemicals by design since they need to maintain their properties throughout the lifetime of the flame retarded product; however, the persistence can be less of a concern for chemicals with a preferable toxicity and bioaccumulation profile. Empirical data for several chemicals identifies them as high or very highly persistent but predicted information identifies them as having low toxicity and/or bioaccumulation hazards.

4. An evaluation of potential combustion by-products was not a hazard category in this alternatives assessment. When considering preferred substitutes, a product manufacturer may wish to consider the types of combustion by-products that may occur when a flame retarded product burns.

In the absence of measured data, we encourage users of this alternatives assessment to be cautious in the interpretation of hazard profiles. Chemicals used at high volumes, or likely to be in the future, should be given priority for further testing. Decision-makers are advised to read the full hazard assessments for each chemical, available in Chapter 4, which may inform whether additional assessment or testing is needed. Contact DfE with any questions on the criteria included in hazard assessments or the thresholds, data, and prediction techniques used to arrive at hazard values (www.epa.gov/dfe).

Where hazard characterizations are based on measured data, there are often cases where the amount of test data supporting the hazard rating varies considerably between alternative chemicals. In Table 4-4 , Table 4-5 and Table 4-6 the hazard characterizations based on SAR or professional judgment are listed in black italics, while those with hazard characterizations based on measured test data are listed in color. The amount of test data behind these hazard characterizations shown in color can vary from only one study of one outcome or exposure, to many studies in many species and different routes of exposure and exposure duration. In some instances, testing may go well beyond basic guideline studies, and it can be difficult to compare data for such chemicals against those with only a single guideline study, even though hazard designations for both chemicals would be considered "based on empirical data" and thus come with a higher level of confidence. Cases where one chemical has only one study but a second chemical has many studies are complex and merit careful consideration. For hazard screening assessments, such as the DfE approach, a single adequate study can be sufficient to make a hazard rating. Therefore, some designations that are based on empirical data reflect assessment based on one study while others reflect assessment based on multiple studies of different design. The hazard rating does not convey these differences – the full hazard profile should be consulted to understand the range of the available data.

6.3 Social Considerations

Decision-makers should be mindful of social considerations when choosing alternative chemicals. This section highlights occupational, consumer, and environmental justice considerations. Stakeholders may identify additional social considerations for application to their own decision-making processes.

Occupational considerations: Workers might be exposed to flame retardant chemicals from direct contact with chemicals at relatively high concentrations while they are conducting specific tasks related to manufacturing, processing, and application of chemicals (see Section 5.1.1). Many facilities have established risk management practices which are required to be clearly communicated to all employees. The National Institute for Occupational Safety and Health (NIOSH) has established a hierarchy of exposure control practices[18]. From best to worst, the practices are: elimination, substitution, engineering controls, administrative controls and personal protection. Switching from high hazard chemicals to inherently lower hazard chemicals can benefit workers by decreasing workplace risks through the best exposure control practices: elimination and substitution of hazardous chemicals. While occupational exposures are different to consumer exposures, workers are also consumers and as such workers are relevant to both exposure groups.

Consumer considerations: Consumers are potentially exposed to flame retardant chemicals through multiple pathways described in Chapter 5. As detailed in Section 5.1.5, exposure research documents that people carry body burdens of flame retardants, including decaBDE and its breakdown products. These findings have created pressure throughout the value-chain for substitution, which impacts product manufacturers. DfE alternatives assessments can assist companies in navigating these substitution pressures.

In recent years there has been a greater emphasis on 'green' products. In addition to substituting in alternative chemicals, some organizations advocate for moving away from certain classes of chemicals entirely (e.g., halogenated flame retardants), with product re-design, to avoid future substitutions altogether. Product manufacturers should be mindful of the role of these organizations in creating market pressure for alternative flame retardant chemicals and strategies, and should choose replacement chemicals – or re-designs – that meet the demands of their customers.

Environmental Justice Considerations: At EPA, environmental justice concerns refer to the disproportionate impacts on minority, low-income, or indigenous populations that exist prior to or that may be created by the proposed action. These disproportionate impacts arise because these population groups experience higher exposures, are more susceptible in response to exposure, or experience both conditions. Factors that are likely to influence resilience/ability to withstand harm from a toxic insult can vary with sociodemographics (e.g., co-morbidities, diet, metabolic enzyme polymorphisms) and are therefore important considerations. Adverse outcomes associated with exposure to chemicals may be disproportionately borne by minority and low income populations. Insights into EPA's environmental justice policy can be accessed

[18] http://www.cdc.gov/niosh/topics/engcontrols/

at: www.epa.gov/compliance/ej/resources/policy/considering-ej-in-rulemaking-guide-07-2010.pdf.

Some populations have higher exposures to certain chemicals in comparison to the average member of the general population. Minority and low-income populations are over-represented in the manufacturing sector, increasing their occupational exposure to chemicals. Higher exposures to environmental chemicals may also be attributable to atypical product use patterns and exposure pathways. This may be due to a myriad of factors such as cultural practices, language and communication barriers, and economic conditions. The higher exposures may also be a result of the proximity of these populations to sources that emit the environmental chemical (e.g., manufacturing industries, industries that use the chemical as production input, hazardous waste sites, etc), access to and use of consumer products that may result in additional exposures to the chemical, or higher employment of these groups in occupations associated with exposure to the chemical.

Some populations are disproportionately exposed to chemicals no longer manufactured in the U.S., including some flame retardants like the components of commercial octa- and pentabromodiphenyl ethers (Zota, Adamkiewicz et al. 2010). Low-income households may have older furniture and other consumer goods, leading to higher exposure to flame retardants as the materials break down over time and chemicals migrate out of products. It is possible that low-income households are less able than higher income households to replace their furniture with new products possibly containing less hazardous materials. Minorities and low income populations tend to live in low income housing, which is typically low quality housing stock and may be poorly ventilated and contain old carpeting, which is a significant source of household dust, and low-income populations may be less able to afford high quality vacuum cleaners to reduce levels of dust in the home. Also, research has documented that certain communities may have greater exposure to industrial waste, making them more exposed to releases from manufacturing facilities (United Church of Christ 1987; Faber and Krieg 2005; Bullard, Mohai et al. 2007; Mohai, Pellow et al. 2009). Finally, certain populations may experience high exposures to toxic chemicals due to geography, food sources, and cultural practices (Burger and Gochfeld 2011). There is research showing that Alaska Natives are disproportionately impacted by certain flame retardants and other persistent organic pollutants, both because of atmospheric transport of persistent chemicals and because of the biomagnification of chemicals in traditional subsistence food webs (Arctic Monitoring and Assessment Program 2009).

Considering environmental justice in the assessment of an alternative chemical may include exploring product use patterns, pathways and other sources of exposure to the substitute, recognizing how upstream factors such as socio-economic position, linguistic and communication barriers, may alter typical exposure considerations. One tool available to these populations is the Toxics Release Inventory (TRI), which was established under the Emergency Planning and Community Right-to-Know Act to provide information about the presence, releases, and waste management of toxic chemicals. Communities can use information reported to TRI to learn about facilities in their area that release toxic chemicals and to enter into constructive dialogue with those facilities. This information can empower impacted populations by providing an understanding about chemical releases and the associated environmental impacts

in their community. Biomonitoring data for the alternative chemical, if available, can also signal the potential for disproportionate exposure among populations with EJ issues.

6.4 Performance Considerations

The DfE approach allows companies to examine hazard profiles of potential replacement chemicals so they can consider the human health and environmental attributes of a chemical in addition to cost and performance considerations. This is intended to allow companies to develop marketable products that meet performance requirements while reducing hazard. This section identifies some of the performance attributes that companies should consider when formulating or selecting a flame retardant, in addition to health and environmental consideration. Performance attributes are critical to the overall function and marketability of flame retardants and should be considered along with other factors. Chapter 2 includes a detailed discussion of the categories of materials, sectors, and products relevant to the chemicals in this assessment, along with a discussion of relevant flammability standards.

The ability of a product to meet required flammability standards is an essential performance consideration for all flame retardant chemicals. The fire safety requirements influence the amount and type of flame retardant, if any, that needs to be added to a resin. Formulations are optimized for cost and performance, so that in some instances it may be equally viable to use a small quantity of an expensive, highly efficient flame retardant or a larger quantity of a less expensive, less efficient chemical.

In addition to flame retardancy properties, the flame-retarded product must meet all required specifications and product standards (e.g., rigidity, compression strength, weight). The polymer/fire retardant combination used in many of the products which contain decaBDE may be complex chemical formulations. In some instances, replacements exist which could allow for relatively easy substitution of the flame retardant. However, a true "drop-in" exchange of flame retardants is rare; some adjustment of the overall formulation, product re-design, or use of inherently flame retardant (IFR) materials is usually required. An alternative with similar physical and chemical properties such that existing storage and transfer equipment as well as flame retardant manufacturing technologies could be used without significant modifications. Unfortunately, chemicals that are closer to being "drop-in" substitutes generally have similar physical and chemical properties, and therefore are likely to have similar hazard and exposure profiles.
Those seeking alternatives to decaBDE should work with flame retardant manufacturers and/or chemical engineers to develop the appropriate flame retardant formulation for their products.

6.5 Economic Considerations

This section identifies economic attributes that companies often consider when formulating or selecting a flame retardant. Economic factors are best addressed by decision-makers within the context of their organization. Accurate cost estimations must be company-specific; the impact of substituting chemicals on complex product formulations can only be analyzed in-house; and a company must determine for itself how changes will impact market share or other business factors. Cost considerations may be relevant at different points in the chemical and/or product lifecycle. These attributes are critical to the overall function and marketability of flame retardants

and flame retarded products and should be considered jointly with performance attributes, social considerations, and human health and environmental attributes.

Substituting chemicals can involve significant costs, as industries must adapt their production processes, and have products re-tested for all required performance and product standards. Decision-makers are advised to see informed chemical substitution decisions as long-term investments, and to replace the use of decaBDE with a chemical they anticipate using for many years to come. This includes attention to potential future regulatory actions motivated by adverse human health and environmental impacts, as well as market trends. One goal is to choose from among the least hazardous options to avoid being faced with the requirement to substitute again.

Flame retardants that are either more expensive per pound or require more flame retardant per unit area to meet the fire safety standards will increase raw material costs. In this situation, a product manufacturer substituting away from decaBDE may pass the cost of a more expensive flame retardant on to customers (e.g., a television manufacturer), who subsequently may pass the cost on to retailers and consumers. In some cases the price premium significantly diminishes over the different stages of the value chain. However, market conditions, competing technologies, and intellectual property issues may influence flame retardant selection when replacing decaBDE.

Handling, disposal, and treatment costs, as well as options for mechanical recycling, may be important considerations when evaluating alternatives. Inherently high hazard chemicals may require special engineering controls and worker protections that are not required of less hazardous alternatives. Disposal costs for high hazard chemicals may also be much higher than for low hazard alternatives. High hazard chemicals may be more likely to result in unanticipated and costly clean-up requirements or enforcement actions should risk management protections fail or unanticipated exposures or spills occur. Also, some chemicals may require specific treatment technologies prior to discharge through wastewater treatment systems. These costs can be balanced against potentially higher costs for the purchase of the alternative chemical. Finally, initial chemical substitution expenses may reduce future costs of mitigating consumer concerns and perceptions related to hazardous chemicals.

It should be noted that, while some assessed alternative chemicals included in this report are currently manufactured in high volume, not all are currently available in quantities that would allow their widespread use immediately. However, prices and availability may change if demand increases.

6.6 Moving Towards a Substitution Decision

As stakeholders proceed with their substitution decisions for decaBDE, the functionality of a product must be maintained with an understanding of the hazard profiles of the chemicals used to meet product performance, and a goal to drive towards safer chemistry on a path of continuous improvement. Substitution decisions may entail evaluating the need for a chemical and whether alternative design and materials may meet the performance needs. When chemical substitution is the necessary approach, the information in this report can help with selection of safer, functional alternatives. The hazard characterization, performance, economic, and social considerations are all factors that will impact the substitution decision. When choosing safer chemicals, alternatives

should ideally have a lower human health hazard, lower ecotoxicity, better degradability, lower potential for bioaccumulation, and lower exposure potential. Where limited data are available characterizing the hazards of potential alternatives, further testing may be necessary before a substitution decision can be made.

Switching to an alternative chemical is a complex decision that requires balancing all of the above factors as they apply to a particular company's cost and performance requirements. DecaBDE is used in a range of polymers and end products; it is therefore unlikely that a single alternative evaluated by this report will fulfill all of the current applications of decaBDE. This report provides hazard information about alternatives to decaBDE to support the decision-making process. Companies seeking a safer alternative should identify the alternatives that may be used in their product (see Table 3-2), and then apply the information provided in this report to aid in their decision-making process.

Alternative chemicals are often associated with trade-offs. For any chemical identified as a potential alternative, some endpoints may appear preferable while other endpoints indicate increased concern relative to the original chemical. A chemical may be designated as a lower concern for human health but a higher concern for aquatic toxicity or persistence. For example, in the case of high molecular weight polymers, where health hazards and potential bioaccumulation are predicted to be low, one trade-off is high persistence. Additionally, there may be limited information about the polymer's combustion byproducts, or how the polymer behaves in the environment and eventually degrades.

Trade-offs can be difficult to evaluate, and such decisions must be made by stakeholders taking into account relevant information about the chemical's hazard, expected product use, and life-cycle considerations. For example, chemicals expected to have high levels of developmental or reproductive toxicity should be avoided for products intended for use by children or women of child-bearing age. Chemicals with high aquatic toxicity concerns should be avoided if releases to water cannot be mitigated. Nonetheless, even when certain endpoints are more relevant to some uses than others, the full hazard profile must not be ignored.

6.7 Relevant Resources

In addition to the information in this report, a variety of resources provide information on regulations and activities that include review or action on flame retardants at the state, national and global levels, some of which are cited in this section.

6.7.1 Resources for state and local government activities

University of Massachusetts at Lowell created a database which "houses more than 700 state and local legislative and executive branch policies from all 50 states from 1990 to the present. The online database makes it simple to search for policies that your state has enacted or introduced, such as those that regulate or ban specific chemicals, provide comprehensive state policy reform, establish biomonitoring programs, or foster "green" chemistry…" (National Caucus of Environmental Legislators 2008).
http://www.chemicalspolicy.org/chemicalspolicy.us.state.database.php

The Interstate Chemicals Clearinghouse (IC2) is an association of state, local, and tribal governments that promotes a clean environment, healthy communities, and a vital economy through the development and use of safer chemicals and products. The IC2 also created a wiki page to allow stakeholders and members of state organizations to share resources for conducting safer alternatives assessments.
http://www.newmoa.org/prevention/ic2/
http://www.ic2saferalternatives.org/

6.7.2 Resources for EPA regulations and activities

EPA's website has a number of resources regarding regulation development and existing regulations, along with information to assist companies in staying compliant. Some of these sites are listed below.

Laws and Regulations
http://www.epa.gov/lawsregs/

Office of Pollution Prevention and Toxics (OPPT): Information on Polybrominated Diphenyl Ethers (PDBEs)
http://www.epa.gov/oppt/pbde/

EPA – OPPT's Existing Chemicals Program
http://www.epa.gov/oppt/existingchemicals/index.html

America's Children and the Environment
http://www.epa.gov/ace/

Integrated Risk Information System (IRIS)
http://www.epa.gov/IRIS/

Design for the Environment Program (DfE)
http://www.epa.gov/dfe

6.7.3 Resources for global regulations

The European Union's REACH (**R**egistration, **E**valuation, **A**uthorisation and Restriction of **Ch**emical substances) legislation was enacted in 2007 and has an "aim to improve the protection of human health and the environment through the better and earlier identification of the intrinsic properties of chemical substances" (European Commission 2011a). Their website contains information on legislation, publications and enforcement.
http://ec.europa.eu/environment/chemicals/reach/enforcement_en.htm

Under REACH, applicants for authorization are required to control the use of Substances of Very High Concern (SVHC). If a SVHC does not have available alternatives, applicants must carry out their own alternatives assessments. The European Chemicals Agency (ECHA) has published a guidance document for this application that provides direction for conducting an alternatives assessment, as well as creating a substitution plan.

http://echa.europa.eu/documents/10162/17229/authorisation_application_en.pdf

The European Union also has issued the Restriction of Hazardous Substances (RoHS) legislation which ensures that new electrical and electronic equipment put on the market does not contain any of the six banned substances: lead, mercury, cadmium, hexavalent chromium, poly-brominated biphenyls PBB or PBDEs above specified levels (European Commission 2011b). http://www.rohs.eu/english/index.html

6.8 The ENFIRO project

ENFIRO, Life Cycle Assessment of Environment-Compatible Flame retardants: Prototypical Case Study (see http://www.enfiro.eu/), is a European Commission FP7 funded research project (Contract-No. 226563 that evaluates viable substitution options for a number of brominated flame retardants for better, safer alternatives (ENFIRO 2011). The consortium is a collaboration between industries, small and medium enterprises and universities. The project delivers a comprehensive dataset on viability of production and application, environmental safety, and a life cycle assessment (LCA) of the alternative flame retardants. Different combinations of the flame retardant with the product are studied in five applications: printed circuit boards, electronic components, injection-molded products, textile coatings, intumescent paint. Three types of halogen free flame retardants (metal-, phosphorous- and nanoclay-based) are investigated in relation to 1) environmental and toxicological risks, 2) viability of industrial implementation, i.e., production of the flame retardant, 3) fire safety, and 4) application of the flame retardant into the material. The fourteen flame retardants that were considered are: aluminum diethylphosphinate, aluminum trihydroxide, ammonium polyphosphate, bisphenol A bis(diphenyl phosphate), resorcinol bis(diphenyl phosphate), triphenyl phosphate, nanoclay, melamine polyphosphate, zinc borate, zinc stannate, zinc hydroxystannate, dihydro oxaphosphaphenantrene oxide, melamine cyanurate, and pentaerythritol. The project approach is based on the chemical substitution cycle in which the alternative flame retardants are evaluated regarding their environmental and toxicological properties, their flame retardant properties, and their influence on the function of products once incorporated. The main objectives of ENFIRO are 1) to deliver a comprehensive dataset on viability of production and application, environmental safety, and a LCA of the alternative flame retardants, and 2) to recommend certain flame retardant/product combinations for future study based on LCA, life cycle costing and risk assessment studies. The outcome of that assessment together with socio-economic information is used in a LCA. The ENFIRO approach and the results are useful for similar substitution studies, e.g., in REACH. An ENFIRO Stakeholder Forum with members representing flame retardant users (e.g., formulators and users of flame retardants, waste (processing) plants) but also from other institutes like non-governmental organizations (NGOs) and policy-related ones, guide the project. This project is set to be completed in August of 2012.

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Appendix A. Additional Reading and Background References

This report is not intended to be a comprehensive resource on all aspects of flame retardant or polymer nanocomposite technology. This section includes additional books and peer-reviewed publications which can provide additional information to the reader.

In many of the polymers which are included in the scope, a synergist is used to enhance the flame retardant performance. An enhancement in flame retardant performance could mean anything from a greater than expected reduction in heat release rate/flame spread rate, to reduced smoke release/afterglow time, to enhanced onset of ignition time/higher ignition temperature. While there are some known specific chemical synergistic interactions in regards to flame retardancy (antimony-halogen, phosphorus-halogen, phosphorus-nitrogen) there are too many to mention them all. Overall, synergism approaches are not as universal as the use of various flame retardants given that synergism is very fire test/polymer/flame retardant chemistry combination specific. Synergism may only be observed in one specific system and not in any others. However, here are some other minor synergisms (including more information below):

- Inorganic enhancement of intumescent chars
- Metal oxides with halogenated FR
- Metal compounds to enhance char formation in polyvinyl chloride (PVC)
- Zinc stannates for enhanced smoke reduction
- Borates with halogenated FR and some char forming FR additives

Similar to flame retardants, polymer nanocomposites can be used in a variety of systems. While polymer nanocomposites act as a nearly universal synergist for lowering polymer flammability, in some cases they may have antagonistic interactions with the other flame retardant, or may bring some other undesirable property change to the final formulation. As with synergists, the number of solutions for decreasing flammability with polymer nanocomposites is vast. Studying the literature is necessary to understand what is possible, probable, and currently unknown.

In addition to the fire retardants being assessed in this document other potential technologies for flame retardancy are listed in the references below. These alternative technologies may not yet be commercially viable, or have not yet been assessed by the EPA DfE program. So while the technology may show an alternate way of providing fire safety to a product, their environmental impact may be unknown. However, the technologies show what is possible and what works, so the reader may be able to develop new fire safe technologies for their product in case other flame retardants are not economically or environmentally viable.

The references are divided into nanocomposite technology and flame retardancy topics below. Most of the references are peer-reviewed papers and there are a few useful books. The field of fire safety is constantly changing and therefore the reader is encouraged to use this list as a starting point to their own literature search.

Polymer Nanocomposite References:

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