Statens forurensningstilsyn
Norwegian Pollution Control Authority

Current State of Knowledge and Monitoring requirements

EMERGING "NEW" BROMINATED FLAME RETARDANTS IN FLAME RETARDED PRODUCTS AND THE ENVIRONMENT

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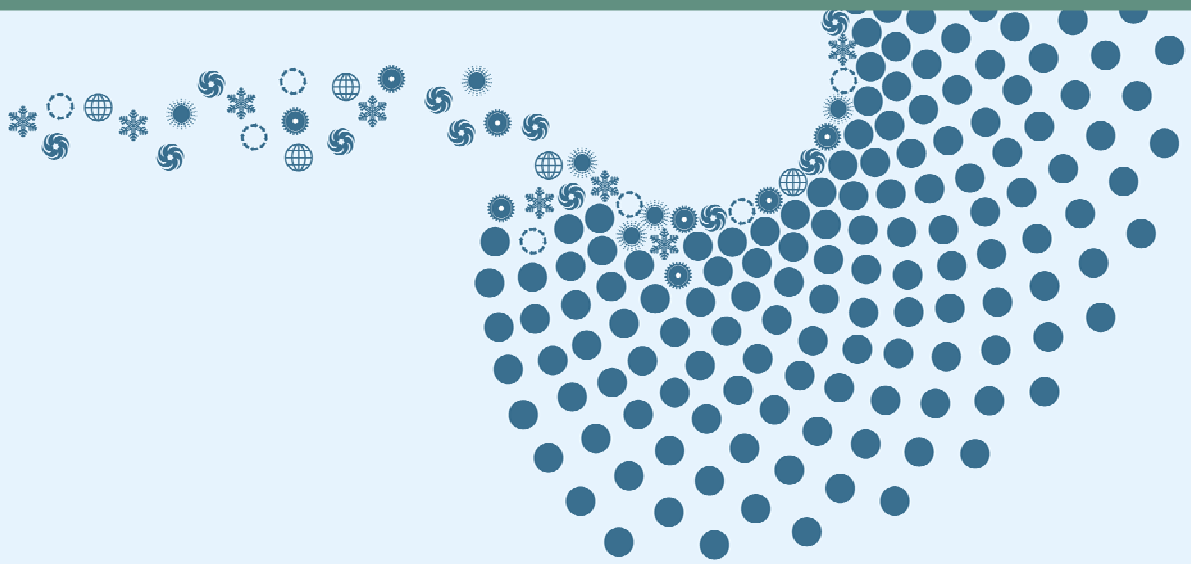

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Current State of Knowledge and Monitoring requirements

Emerging “new” Brominated flame retardants in flame retarded products and the environment

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NILU Report no: OR 16/2009
ISBN: 978-82-425-2091-3 (T)
ISBN: 978-82-425-2092-0 (E)

Preface

Brominated flame retardants are a group of chemicals that inhibit combustion. They are extensively used in electrical and electronic equipment, transport equipment, building materials, paint and insulation foams. However, many of the brominated flame retardants have undesirable effects on the environment and on human health. Therefore it is a nationnal target to substantially reduce the release of five prioritized brominated flame retardants before 2010 and completely eliminate the discharge of these five substances before 2020.

The overall aim of this study is to perform a review of the current state of the knowledge on emerging “new” brominated flame retardants. This includes the use of the selected substances, environmental levels, data on toxicity and ecotoxicity, potential to bioconcentrate and bioaccumulate in the food web, analytical possibilities, potential for long range transport and their persistence in the environment. Further, this information is used to select compounds that based on the current knowledge can be relevant for further monitoring.

The Norwegian Pollution Control Authority (SFT) has commissioned the environmental research institute NILU (Norway), Swerea IVF (Sweden) and WECC Wania Environmental Chemist Corp. (Canada) to perform this study.

SFT, Oslo, December 2008

Sigurd Tremoen
Director of the Department of Chemicals and Local Environmental Management

Contents

1. Summary

This report summarises the current state of knowledge on types, market volumes, manufacturers and uses of brominated flame retardants, with tables containing currently available data on the applications, uses, producers and suppliers of these BFRs. The accumulated knowledge of their physicochemical properties, potential health and environmental effects, eg. acute toxicity, ecotoxicity, bioaccumulation, degradation and fate, environmental levels and potential for long range transport is also summarised.

The report concludes with a summary of the current sampling and analysis techniques and finally the prioritization; giving a table with the selected priority compounds and Appendix I which contains the information summary of compound specific data and estimated environmental properties as a basis for making the priority selection.

Current production volumes for these BFRs are largely unknown and most data available is outdated. The approach was to estimate the production volumes based on known production volumes for TBBP-A and PBDEs and HBCDD. We estimated the worldwide total volume of the 21 new flame retardants and other BFRs is around 100000 metric tonnes per year.

Limited data is available on toxicity, ecotoxicity, endocrine effects, and the absorption, distribution and excretion and bioaccumulation/concentration processes of these 21 “new” BFRs. Three BFRs lack, to our knowledge, any relevant information published in the peer reviewed literature.

The potential for these selected BFRs to be subjected to long range transport (LRT) was studied. Results showed that dibrominated styrenes (CAS 31780-26-4, 125904-11-2), 2,4,6-tribromophenyl allyl ether (CAS 3278-89-5) and pentabromobenzyl acrylate (CAS 59447-55-1) - based on their partitioning properties alone - were judged to have the potential to undergo LRT. However, estimated short atmospheric half life indicates that they are more likely to pose a problem in the near source environment, especially if they should be recalcitrant to biotransformation. A valid concern is whether pentabromobenzyl acrylate may form a persistent and potentially bioaccumulative metabolite.

The substances that have partitioning properties that suggests LRT and are predicted to be fairly persistent are the highly brominated monoaromatics, such as hexabromobenzene, pentabromotoluene, and pentabromoethylbenzene. The predicted LRT behaviour is comparable to those of established POPs, although these predictions may be overestimated because the LRT assessment does not include the possibility of photolytic debromination.
Some of the heavier BFRs, such as Decabromodiphenylethane (CAS 84852-53-9), have structures not unlike those of decaBDE, and may be subject to similar long range transport and bioaccumulation processes.

12 of the 21 “new” BFRs that were under investigation was listed as potentially relevant for further investigation and monitoring in the Norwegian environment. In addition, 2,3-dibromopropyl -2,4,6-tribromophenyl ether (BPTE) and 2-ethylhexyl-2,3,4,5-tetrabromobenzoate (TBB) was added to the list. BPTE

was selected as it is the main component of bromkal 73-5PE, and a propable reductive precursor of the priority compound; 2,4,6-Tribromophenyl allyl ether. In addition, BPTE was one of the more prominent compounds in seal from the Barents Sea. TBB was selected as this is one of the major compounds in Firemaster 550 together with the priority compound Bis(2-ethylhexyl)tetrabromophtalate (TBPH).

Reports on the environmental screening of these "new" BFRs are scarce. Assuming that several new BFRs behave in a similar manner to known BFRs, future screening should be prioritized in similar "hot spots" and reference sites as for the well known prioritized BFRs, like penta-, octa- and deca-BDEs, TBBP-A and HBCDD. Examples of this are; electronic dismantling plants, areas where the industry have current use of these type of BFRs, landfills, waste water treatment plants, domestic and working environments.

It was only possible to locate good national or international assessments on a few selected BFRs, and many data were found in old and not easily accessible documents. The validity of these tests varies and can often not be evaluated. A thorough evaluation of each BFR was thus not possible within the limits of this project.

Project leader: Mikael Harju
Authors: Eldbjørg S. Heimstad, Dorte Herzke, Torkjel Sandanger, Stefan Posner and Frank Wania

Acknowledegements
The authors would like to thank Hildegun Hammer, Silje Klaussen, Kari Kvamsdal and Morten Moe for their much appreciated help with language, layout, literature search, collection of data and formatting.

2. Sammendrag

Denne rapporten oppsummerer kunnskapsstatus for såkalte "nye" bromerte flamme hemmere (BFH) ved å samle all tilgjengelig vitenskapelig informasjon om, samt evaluere bruken av disse kjemikaliene i dag. Type innsamlet data er; markedsvolum, produsenter, leverandører anvendelsesområder, og bruk av BFH. Kunnskapsstatus for fysikalsk-kjemiske egenskaper, potensielle helse og miljø effekter som akutt toksisitet og økotoksisitet, bioakkumulering, degradering, skjebne i miljøet og mulighet for at disse forbindelsene kan langtransporteres, er også rapportert.
I konklusjonen er det laget en liste over potensielle forbindelser som er aktuelle for fremtidig miljøundersøkelsert. Her er det også samlet informasjon om prøvetakingsprosedyrer og analytiske metoder (Appendix 1).
Oppdaterte produksjonstall for disse mindre kjente BFH er lite tilgjengelig og det meste av data er derfor utdatert. Estimater er gjort på bakgrunn av kjente produksjonsvolumer for TBBP-A, PBDE og HBCDD. Det globale totalvolumet for de 21 BFH i dette studiet og ukjente BFH, er estimert til å være ca 100 000 tonn per år.
Det er en begrenset mengde data tilgjengelig på toksisitet, økotoksisitet, endokrine effekter og prosesser rundt absorbsjon, distribusjon og bioakkumulasjon/konsentrasjon av disse 21 forbindelsene. For tre av forbindelsene, er det etter det vi kjenner til, ikke publisert relevant informasjon i forhåndsevaluerte tidskrifter. Basert på fasefordelingsegenskaper, ble følgende forbindeler vurdert til å ha langtransportpotensialet (LRT); dibrom-erte styrener (CAS 31780-26-4, 125904-11-2), 2,4,6-tribromofenylallyleter (CAS 3278-89-5) og pentabromobenzylakrylat (CAS 59447-55-1). Kort halveringstid gjør det derimot mer sannsynlig at disse forbindelsene blir et miljøproblem nært kilden. Det er også grunn til å være oppmerksom på mulige bioakkumulerende metabolitter av pentabromobenzylakrylat.

Forbindelser som har fasefordelingsegenskaper som skulle tilsi LRT og persistens i miljøet, er de høyt bromerte monoaromatene, som heksabrombensen, pentabromtoluen og pentabrometylbensen. Kalkulerte LRT verdier er sammenlignbare med tradisjonelle POPer, men verdiene kan være noe overestimerte i og med at det ikke er tatt hensyn til atmosfærisk nedbrytning.

Noen av de tyngre BFH som Dekabromodifenyletan (CAS 84852-53-9), har strukturer som ikke er helt ulik deka-BDE, noe som indikerer muligheten for lignene LRT mekanismer og evne til bioakkumulering.

Basert på de tidligere nevnte kriteriene ble 12 av de 21 forbindelsene vurdert som relevante for videre undersøkelser og monitorering i det norske miljøet. I tillegg ble 2,3-dibromopropyl-2,4,6-tribromofenyleter (BPTE) og 2-etylheksyl-2,3,4,5-tetrabromobenzoat (TBB) lagt til denne listen. BPTE ble valgt siden den er en av hovedforbindelsene i Bromkal 73-5PE, og en sannsynlig reduktiv prekursor til forbindelsen 2,4,6-Tribromofenylallyl-eter. I tillegg var BTPE en av de dominerende forbindelsene funnet i sel fra Barentshavet. TBB ble valgt som en av hovedkomponentene i Firemaster 550 sammen med den prioriterte Bis(2-etylheksyl)tetrabromoftalat (TBPH).
Det finnes bare begrensede data på allerede utførte screeninger av de 12 BFHe-

ne i miljøet. Dersom man antar at flere av disse nye BFH oppfører seg likt i miljøet som kjente BFH, kan det være relevant å lete etter disse nye BFH på kjente såkalte ”hotspots” og referansestasjoner. Dette for å kunne sammenligne med data på allerede studerte BFH (PBDE, TBBP-A og HBCDD) og dermed kunne sammeligne skjebne og livsløp i miljøet. Eksempler på slike ”hotspots” og referansestasjoner er: retur-stasjoner for elektronikk, industrielle områder hvor BFH er i bruk, fyllplasser, renseanlegg, arbeids- og hjemmemiljø.
Kun for ett fåtall av de aktuelle forbindelsene var det mulig å samle gode nasjonale og internasjonale rapporter, og mye data er funnet i gamle og ikke lett tilgjengelige dokumenter. Slik informasjon er ofte vanskelig å etterprøve og validere. En grundig gjennomgang av alle BFH i dette studiet var derfor ikke mulig innefor et prosjekt av denne størrelsen.

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Forfattere: Eldbjørg S. Heimstad, Dorte Herzke, Torkjel Sandanger, Stefan Posner and Frank Wania

Tusen takk til: Hildegun Hammer, Silje Klaussen, Kari Kvamsdal og Morten Moe for hjelp med språk, datainnsamling, litteratursøk, oppsett og formatering av dokumentet.

3. Introduction

Flame retardants can be divided into the inorganic and organic halogenated and organophosphate compounds.

Inorganic flame-retardants include metal hydroxides such as aluminium hydroxide and magnesium hydroxide, and ammonium salts. As a group, these flame retardants represent the largest fraction of total flame retardants in use.

Halogenated flame retardants are primarily based on chlorine and bromine. Typical halogenated flame retardants are halogenated paraffin's, halogenated alicyclic and aromatic compounds and halogenated polymeric materials. Halogenated flame retardants also often contain other heteroelements, such as phosphorus or nitrogen. These flame retardants react with flammable gases to slow or prevent the burning process.

Halogenated flame-retardants can be divided into three classes:

- ***Aromatic***, which includes the major brominated flame retardants, tetrabromobisphenol A (TBBP-A) and decabromodiphenylether (decaBDE).
- ***Cycloaliphatic,*** including the hexabromocyclododecane (HBCDD) isomers.
- ***Aliphatic***, globally representing a minor group of substances.

Inorganic flame retardants are added as fillers into the polymer and are considered immobile in contrast to the organic additive flame retardants. The whole group of inorganic flame retardants represents around 50 % by volume of the global flame retardant production, mainly as aluminium trihydrate, which is in volume the biggest flame retardant category in use on the market.

Flame-retardants are either additive or reactive. Reactive flame-retardants are added during the polymerisation process and become an integral part of the polymer, forming a co-polymer. The result is a modified polymer with flame retardant properties and different molecular structure compared to the original polymer molecule. This prevents them from leaving the polymer and keeps the flame retardant properties intact over time with very low emissions to the environment (Danish EPA, 1999). Reactive flame-retardants are mainly used in thermosets, especially polyester, epoxy resins and polyurethanes (PUR) in which they can be easily incorporated (Posner, 2006).

Additive flame retardants are incurporated into the polymer prior to, during, or more frequently after polymerization. They are used especially in thermoplastics. If they are compatible with the plastic they act as plasticizers, otherwise they are considered as fillers. Additive flame-retardants are monomer molecules that are not chemically bound to the polymer. They may therefore be released from the polymer and thereby also discharged to the environment.

Several types of halogenated flame retardants, mainly brominated flame retardants, are described in the literature. This includes compounds belonging to families of polybrominated diphenylethers (PBDEs), tetrabromobisphenol-A (TBBPA) and its derivatives, such as tetrabromobisphenol A

bis(dibromopropyl ether) and tetrabromobisphenol A bis (allyl ether), tribromophenol (TBP) and brominated phthalic anhydride. Use of flame retardant additives depends mainly on the type of polymer to be flame retarded. Although the use of halogenated flame retardants is strongly questioned due to their potentially harmful environmental and health characteristics they represent around 25% by volume of the total global production of flame retardants with a growth of around 5% per year (Fink et al., 2005).

3.1 Estimated market volumes

Limited information is available on the current global market volume on emerging brominated flame retardants. In order to get a fair picture of current volumes that may be used today especially less known brominated flame retardants such as those reviewed in this report, it is nessecary to assess possible volumes estimated from better known volumes of TBBP-A, PBDEs and HBCDD. It is assumed that the volume left might represent the less known brominated flame retardants reviewed in this report. It should be clear that these assumptions are rough and gives only a fair estimate of possible volumes that might be on the market. The latest independent figures represented are more than 15 years old (WHO, 1994) and are not credible anymore.

Brominated compounds represent approximately 20 to 25 percent by volume of the global flame retardant production. Table 1 show the total global use of flame retardants in 2005 whith a total use of brominated flame retardants of 311 000 metric tonnes which would be around 21% of the total consumption of flame retardants (Fink et al., 2005).The current total amount of TBBP-A produced worldwide is estimated to 150000 tonnes/year according to figures from the European commission (JRC, 2006). Arias reported that world-wide demand for decabromodiphenyl ether was 54800 tonnes/year in 1999 (Arias, 2001).

If we assume that the production volumes of TBBP-A and decaBDE have not changed dramatically over the past few years, the figures in Table 1 suggest that all other BFRs are produced and used in volumes up to 130.000 metric tonnes[1] per year or maybe slightly more. A fair estimate would be a total volume of around 100000 metric tonnes per year in total for the 21 new flame retardants, possibly including also other brominated flame retardants that are not within the scope of this study.

3.2 Applications and uses of „new“ flame retardants

With the increasing use of thermoplastics and thermosets on a large scale for applications in buildings, transportation, electrical engineering and electronics, a variety of flame-retardant systems have been developed over the past 40 years. Table 2 gives an overview of materials where the “new” flame retardants may occur (WHO, 1997;Posner, 2006;Troitzsch, 2007).

[1] Estimated total volume of the new brominated flame retardants = 311.000 tonnes – 150.000 tonnes (TBBP-A) – 30.000 tonnes (decaBDE) = 130.000 tonnes per year.

Table 1. Global consumption of flame retardants and their geographical distribution (Fink et al., 2005).

Category	**United States**	**Europe**	**Japan**	**Other Asia**	**Total volume [1000 metric tonnes]**	**Value [million USD]**
Aluminium hydrox-ide	315	235	47	48	645	424
Organo phosphorous FRs	65	95	30	14	205	645
Brominated FRs	***66***	***56***	***50***	***139***	***311***	***930***
Antimony trioxide	33	22	17	44	115	523
Chlorinated FRs	33	35	5	10	82	146
Other FRs	51	47	11	14	123	197
TOTAL	**564**	**489**	**160**	**269**	**1481**	**2865**

[2]

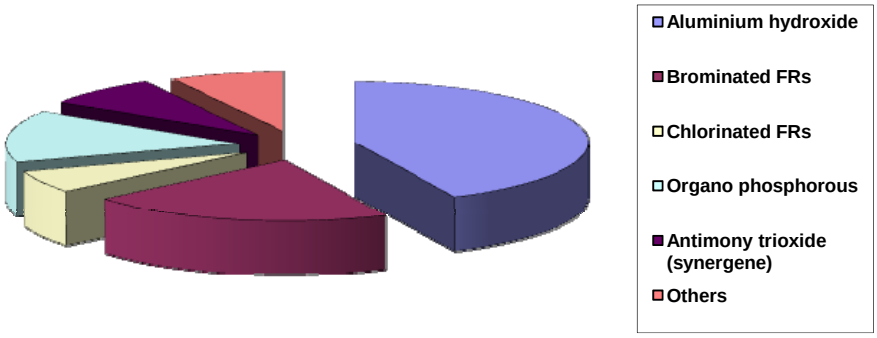


Figure 1. The global market share of groups of flame retardants (Fink et al., 2005)

[2] Kirschner M, personal communication (2008)

Table 2. Possible occurrence of the "new" flame retardants in various materials.

Substance	**CAS**	**Type of BFR**	**Materials where applied**
Decabromodiphenylethane	84852-53-9	Additive	Styrene
Hexabromobenzene	87-82-1	N/A	N/A
1,2-Bis(2,4,6-tribromophenoxy)ethane	37853-59-1	Additive	Thermoplastics, Acrylonitrile butadiene styrene terpolymer (ABS), High impact polystyrene (HIPS)
Pentabromoethylbenzene	85-22-3	Additive	Unsaturated polyesters, styrene butadiene copolymers, textile
Pentabromotoluene	87-83-2	N/A	Unsaturated polyesters, polyethylene, polypropylenes,polystyrene, SBR-latex, textiles, rubbers, ABS
Pentabromobenzyl acrylate Poly(pentabromobenzyl) acrylate	59447-55-1 (as monomer) 59447-55-1 (as polymer)	Reactive Intermediate Polymer	Polybutyleneterephatlate (PBT), Polyethylene terephatale (PET), ABS polypropylene, Polystyrene and others - polyamides, polyesters, polycarbonates, Polyamide
Ammonium bromide	12124-97-9	Filler	Wood
2,4,6-tris(2,4,6-tribromophenoxy)-1,3,5-triazine	25713-60-4	N/A	N/A
Tris(tribromoneopentyl) phosphate	19186-97-1	Additive	Styrene, Polyurethane
1-Propanol, 2,2-dimethyl-, tribromo derive. or Tribromoneopentylalcohol	36483-57-5 1522-92-5	Reactive intermediates	Polyurethane, Rigid and flexible polyurethane foam
Dibromoneopentyl glycol	3296-90-0	Reactive intermediates	Unsaturated polyesters, elastomers Rigid polyurethane foams
2,4,6-tribromophenol	118-79-6	Reactive intermediates	Epoxy resins, phenolic resins, polyester resins, polyolefins

Ethylene bistetrabromo phthalimide	32588-76-4	Additive	High Impact polystyrene, polyethylene, polypropylene, thermoplastic polyesters, polyamide, EPDM; rubbers, polycarbonate, ethylene co-polymers, ionomer resins, textiles
1,4-Bis(pentabromophenoxy) tetrabromobenzene	58965-66-5	Reactive intermediate	Engineering thermoplastics
Tetrabromophthalic anhydride	632-79-1	Additive, Reactive intermediates for polyols, esters and imides	Unsaturated polyesters and rigid polyurethane foams, paper, textiles, Epoxides, wool
Tetrabromobisphenol A bis (allyl ether)	25327-89-3	Additive Reactive	EPS, foamed polystyrene
Bis(2-ethylhexyl) tetrabromophthalate	26040-51-7	Additive	PVC, Neoprene
Tetrabromobisphenol A (2,3-dibromopropyl ether)	21850-44-2	Additive	Polyolefine resins Polystyrene
2,4,6-Tribromophenyl allyl ether	3278-89-5	Reactive	Expandable polystyrene (EPS), Polystyrene foam
Dibromostyrene	31780-26-4	N/A	Styrenic polymers, engineering plastics
1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol or 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester	77098-07-8 20566-35-2	N/A	N/A

N/A : not available or not applicable

It needs to be understood that each flame retardant application is specific and unique, and there is no single universal solution for fire protection of materials and applications.

Table 3 show a range of possible applications with address to Table 2, where the "new" flame retardants may occur.

Table 3. Possible applications of the "new" brominated FRs in various materials and processes.

Materials/polymers/resins	**Applications**	**Commercial commodities for the applications**
Epoxy resins	Circuit boards, protective coatings	Computers, ship interiors, electronic parts
Polyvinylchloride (PVC)	Cable sheets	Wires, cables, floor mats, industrial sheets
Polyurethane (PUR)	Cushioning materials, packaging, padding	Furniture, sound insulation packaging, padding panels, wood imitations, transportation
Unsaturated (Thermoset) polyesters (UPE)	Circuit boards, coatings	Electrical equipment, coatings coatings for chemical processing plants, mouldings, military and marine applications: construction panels.
Acrylonirile-butadiene- styrene-terpolymer (ABS)	Electronics	Housings for business machines, dashboards, toys, equipments for refrigerator, telephones, and other consumer electronics
High Impact Polystyrene (HIPS)	Electronics	Housings of electronic products, wiring parts
Rubber	Transportation	Conveyor belts, foamed pipes for insulation
Butyl styrene-based rubber (SBR)	Transportation	Conveyor belts, foamed pipes for insulation
Textiles	Coatings	Back coatings and impregnation for carpets, automotive seating, furniture in homes and official buildings, aircraft, underground

Their occurrence should be seen in the light of market or legislative fire requirements set on these applications. If the fire requirements are not met, there is no market for the individual supplier and the manufacturer. On the other hand, there are no prescriptive fire requirements stipulating that particular

flame retardants have to be used to meet the requirements. Conclusively there is no point to assume any occurrence of any of these 21 flame retardants or other flame retardants, where there is no demand for fire requirements at all.

3.3 Producers and suppliers on the international market

A handful of producers of brominated flame retardants operates internationally. Table 4 gives an overview of producers and importers to the EU.

Table 4. Overview of producers and importers of the "new" flame retardants (ESIS, 2008).

Substance (all synonymes)	**CAS**	**Estimated volumes**	**EU-importer**	**Producer**
Decabromodiphenylethane	84852-53-9	N/A	N/A	Albemarle
Hexabromobenzene	87-82-1	N/A	N/A	N/A
1,2-Bis(2,4,6-tribromophenoxy)ethane	37853-59-1	LPV	Dow Chemicals	Chemtura
Pentabromoethylbenzene	85-22-3	LPV		Albemarle
Pentabromotoluene	87-83-2	LPV	Eurobrom B.V	
Pentabromobenzyl acrylate	59447-55-1	LPV	Eurobrom B.V	Dead Sea Bromine group
Ammonium bromide	12124-97-9	HPV	Albemarle	Dead Sea Bromine group
2,4,6-tris(2,4,6-tribromophenoxy)-1,3,5-triazine	25713-60-4	N/A	N/A	Dead Sea Bromine group
Tris(tribromoneopentyl) phosphate	19186-97-1	N/A	Unibrom	Dead Sea Bromine group
1-Propanol, 2,2-dimethyl-, tribromo derive. (Tribromoneopentylalcohol)	36483-57-5	N/A	N/A	Dead Sea Bromine group
Dibromoneopentyl glycol	3296-90-0	LPV	Enichem Italy Eurobrom BV	Dead Sea Bromine group
2,4,6-tribromophenol	118-79-6	HPV	Eurobrom BV	Dead Sea Bromine group
Ethylene bistetrabromo phthalimide	32588-76-4	HPV	Great Lakes Europe	Albemarle

			Sylachim division Sochibo	
1,4-Bis(pentabromophenoxy) tetra-bromobenzene	58965-66-5	LPV	N/A	Albemarle
Tetrabromophthalic anhydride	632-79-1	LPV	Great Lakes Europe Sylachim division Sochibo	Chemtura
Tetrabromobisphenol A bis (allyl ether)	25327-89-3	LPV	Great Lakes Europe	Chemtura
Bis(2-ethylhexyl) tetrabromophthala-te	26040-51-7	LPV	Great Lakes Europe	Chemtura
Tetrabromobisphenol A (2,3-dibromopropyl ether)	21850-44-2	LPV	Great Lakes Europe Riedel de Haen AG Germany	Dead Sea Bromine group
2,4,6-Tribromophenyl allyl ether	3278-89-5	LPV	Eurobrom BV	Chemtura
Dibromostyrene	31780-26-4	N/A	N/A	Chemtura
1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethy-lene glycol and propylene glycol or 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester	77098-07-8 20566-35-2	N/A	N/A	Chemtura

N/A : not available or not applicable; LPV: Low volume production
HPV: High volume production

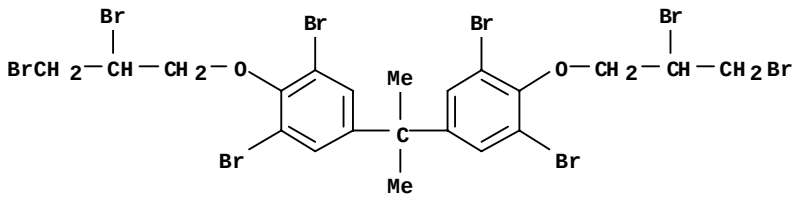
4. Current knowledge on selected BFRs

Reviewers have categorized the chemistry of flame retardants in an assortment of ways but for the purpose of this project three generic categories have been used (aromatics, aliphatics and inorganics). These are further divided into subgroups as to simplify the overview of the material as each subheading of chemicals generally has similar physicochemical characteristics and use.

4.1 Aromatics

4.1.1 Tetrabromobisphenol A derivatives

4.1.1.1 Tetrabromobisphenol A bis(2,3-dibromopropyl ether)



Characteristics of the compound:

CAS No.:	21850-44-2
CA Index name:	Benzene, 1,1'-(1-methylethylidene)bis(3,5-dibromo-4-(2,3-dibromopropoxy)-
Molecular Formula:	C21 H20 Br8 O2
Molecular Weight (g/mol)	943.61[a]
Melting Point/range (°C)	90-105[b], 90-100[c]
Boiling Point/range (°C)	676.5±55.0[a]
Vapour Pressure (Pa (25°C))	1.60E-07[a]
Water Solubility (g/l (25°C))	1.60E-07[a]
Partition Coefficient (log P_{ow})	10.422±0.696[a]
Partition Coefficient (log K_{oc})	7.00[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Data from SciFinder data base originating from experimentally determined properties
c) Data from the WHO report: "Environmental health criteria 172. Tetrabromobisphenol A and derivatives" experimental data (WHO, 1995)

Known uses: This chemical is marketed as SAYTEX HP-800A, HP-800AG, and HP-800AGC by Albemarle Corp.; PE-68 by Great Lakes Chemical Corp. for use in HIPS; and in product 403AF by LG Chem with use in fire retarded HIPS. However, this flame retardant is mainly used in other polymers including polypropylene (Ecology, 2006).

Synonyms: Propane, 2,2-bis[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]- (8CI); 1,1'-Isopropylidenebis[3,5-dibromo-4-(2,3-dibromopropoxy)benzene]; 2,2-Bis[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]propane; 2,2-Bis[4-(2,3-dibromopropoxy)-3,5-dibromophenyl]propane; 2,2-Bis[4-(2,3-dibromopropyloxy)-3,5-dibromophenyl]propane; 2,2-Bis[[3,5-dibromo-4-(2,3-dibromopropyloxy)]phenyl]propane; 3,3',5,5'-Tetrabromobisphenol A bis(2,3-dibromopropyl) ether; 4,4'-Isopropylidenebis[2,6-dibromo-1-(2,3-dibromopropoxy)benzene]; Bis(2,3-dibromopropoxy)tetrabromobisphenol A; Bromkal 66-8; D 5532; FG 3100; FR 720; Fire Guard 3100; Flame Cut 121K; Flame Cut 121R; GX 5532; PE 68; PE 68 (fireproofing agent); Pyroguard SR 720; SR 720; Saytex HP 800AG; TBBPA-DBPE; Tetrabromobisphenol A 2,3-dibromopropyl ether; Tetrabromobisphenol A bis(2,3-dibromopropyl ether).

Human Exposure: No data available.

Toxicity: The acute LD_{50} for mice was > 20 g/kg when given in feed and observed for 14 days. The acute dermal LD_{50} for mice was > 20 g/kg when applied to closely clipped intact skin for 24 hours and then observed for 14 days (WHO, 1995).
Mice were administered levels of 200 or 2000 mg/kg per day in their diet for 90 days. At the end of the study, no deaths had occurred at either level. No abnormal symptoms were observed in the pathological examination (WHO, 1995). Low sub-chronic NOAEL = 200 mg/kg (Pakalin et al., 2007). Tetrabromobisphenol A bis(2,3-dibromopropyl ether) (TBBPA-DBPE) did not show any immunotoxic effect, in vitro, on the splenocytes of C57BL/6 mice (Pullen et al., 2003).

Eye/skin irritation: No data available.

Genotoxicity: The National Toxicology Program (NTP) believe that the substance might have a carcinogenic potential (Pakalin et al., 2007).

Endocrine effects: No endocrine effects was observed by TBBPA-DBPE on the steroidogenic enzyme aromatase (CYP19 or CYP17) in H295R human adrenocortical carcinoma cells in culture (Canton et al., 2003;Canton et al., 2006). No greater endocrine effects were observed for TBBPA-DBPE on the arylhydrocarbon receptor, androgen receptor, progesterone receptor, and estrogen receptor. TBBPA-DBPE has a high potential to inhibit the estradiol sulfotransferase and have a moderate competition with the thyroxine for the binding to the plasma transport protein transthyretrin. Results showed that TBBPA-DBPE have similar but a magnitude lower effect on sulfotransferase and transtyrethrin assays as tetrabromobisphenol A, but it cannot be excluded that contaminants of tetrabromobisphenol A in the TBBPA-DBPE standard is responsible for this effect (Hamers et al., 2006).

Absorption, distribution and excretion: Absorption, distribution, metabolism and excretion was studied by oral and i.v. administration in rats. TBBPA-DBPE was shown to be largely excreted in feces (95 %). The conclusion was that TBBPA-DBPE is poorly absorbed through the gastrointestinal tract and the amount that is absorbed accumulates in the liver and is slowly metabolized and

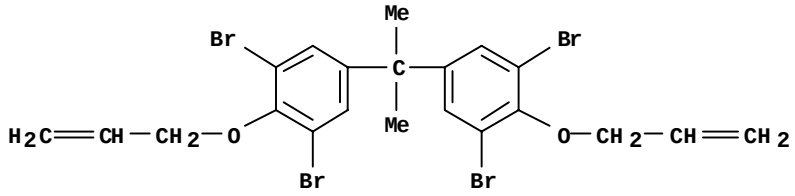
eliminated in the feces (Knudsen et al., 2007).

Bioaccumulation, degradation and fate: Biodegradation tests have shown a negative response, and accumulation in carp was judged to be very small showing that TBBPA-DBPE might not be readily biodegradable (WHO, 1995). Experimental studies on the hydrolysis of environmental contaminants showed TBBPA-DBPE to be susceptible to hydrolysis, at the same level as DDT with an experimental half-life of < 0.02 hours at 273K (Methanol/DMF, 5/95 ratio) with sodium methoxid as a strong nucleophile. The elimination product, TBBPA bis(bromopropenyl ether), might be the more prevalent compound in sediments in a similar manner as DDE is for DDT (Rahm et al., 2005).

Environmental levels: TBBPA-DBPE at a concentration of 1.3 ng/g dust wt where identified in dust collected near an artificial stream and pond system in Berlin, Germany (Sawal et al., 2008).

Emissions and monitoring data from the Nordic countries: No data available.

4.1.1.2 Tetrabromobisphenol A diallyl ether



Characteristics of the compound:

CAS No.:	25327-89-3
CA Index name:	Benzene, 1,1'-(1-methylethylidene)bis[3,5-dibromo-4-(2-propen-1-yloxy)-
Molecular Formula:	C21 H20 Br4 O2
Molecular Weight (g/mol)	624.00[a]
Melting Point/range (°C)	118-120[b], 115-120[c]Boiling
Point/range (°C)	525.0±50.0[a]
Vapour Pressure (Pa (25°C))	1.83E-08[a]
Water Solubility (g/l (25°C))	1.60E-05[a]
Partition Coefficient (log P_{ow})	8.539±0.614[a]
Partition Coefficient (log K_{oc})	6.02[a]

a) Data from the SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Data from the SciFinder data base originating from experimentally determined properties
c) Data from the WHO report: "Environmental health criteria 172. Tetrabromobisphenol A and derivatives" experimental data (WHO, 1995)

Known uses: Tetrabromobisphenol A diallyl ether (TBBPA-diallylether) is used as a reactive flame retardant in polystyrene foams (WHO, 1995).

Synonyms: Benzene, 1,1'-(1-methylethylidene)bis[3,5-dibromo-4-(2-propenyloxy)- (9CI); Propane, 2,2-bis[4-(allyloxy)-3,5-dibromophenyl]- (8CI); 1,1'-Isopropylidenebis[4-(allyloxy)-3,5-dibromobenzene]; 2,2-Bis(3,5-dibromo-4-allyloxyphenyl)propane; 2,2-Bis(4-allyloxy-3,5-dibromophenyl)propane; BE 51; FG 3200; Fire Guard 3200; Flame Cut 122K; Pyroguard SR 319; SR 319; Tetrabromobisphenol A allyl ether; Tetrabromobisphenol A bis(allyl ether).

Human Exposure: No data available.

Toxicity: TBBPA-diallylether showed no dermal or acute oral toxicity of rats using single doses of up to 5.0 g/kg or to 1 g/kg/day in the feed for 28 days. The acute inhalation LC_{50} in rats was 13.4 mg/l. TBBPA-diallylether gavage exposure of pregnant rats from gestation days 6 through 15 caused no maternal toxicity and was not embryotoxic, fetotoxic, nor teratogenic (TOXNET, 2008). In a report the WHO concludes that, based on the available data, the acute oral and dermal toxicities of this compound are low (WHO, 1995).

Eye/skin irritation: TBBPA-diallylether is a mild eye irritant, and slightly irritating to the skin of rabbits (WHO, 1995).

Genotoxicity: No genetic activity was seen in the Ames Salmonella/microsome plate assays in the presence or absence of Aroclor-induced rat liver homogenate (TOXNET, 2008).

Endocrine effects: A study of the immunotoxic effects of BFRs using splenocytes of mice and incubating them with TBBPA-diallylether showed to significantly inhibit the expression of Interleukin-2 receptor alfa-chain suggesting that TBBPA-diallylether is a potential immunotoxin (Pullen et al., 2003).

Absorption, distribution and excretion: No data available.

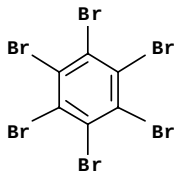
Bioaccumulation, degradation and fate: Experimental studies on the hydrolysis of environmental contaminants showed TBBPA-diallyl ether not to be easily hydrolysed, with an experimental half-life of > 240 hours at 333 K (Methanol/DMF, 0.5/99.5 ratio) with sodium methoxid as a strong nucleophile. This suggests that TBBPA-bis(diallyl ether) might be resistant to environmental degradation (Rahm et al., 2005).

Environmental levels: No environmental levels of TBBPA-diallyl ether is published in the peer reviewed literature.

Emissions and monitoring data from the Nordic countries: No data available.

4.1.2 Monoaromatics

4.1.2.1 Hexabromobenzene



Characteristics of the compound:

CAS No.:	87-82-1
CA Index name:	Benzene, 1,2,3,4,5,6-hexabromo-
Molecular Formula:	C6 Br6
Molecular Weight (g/mol)	551.49[a]
Melting Point/range (°C)	327[b], 326-327[c], 326[d]
Boiling Point/range (°C)	417.5 ± 40[a]
Vapour Pressure (Pa (25°C))	1.14E-04[a] 3.17E-04 (liquid subcooled)[d] 7.5E-04 (liquid subcooled)[c]
Water Solubility (g/l (25°C))	7.70E-04[a], 1.10E-07[d], 3.0E-06[c]
Partition Coefficient (log P_{ow})	5.851±0.674[a], 6.07d
Partition Coefficient (log K_{oc})	4.56[a]

a) Data from the SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Data from the SciFinder data base originating from experimentally determined properties
c) Experimental results from Tittlemier et al. (Tittlemier et al., 2002)
d) Experimental results from Kawamoto and Kuramochi (Kawamoto and Kuramochi, 2007)

Known uses: No data found.

Synonyms: Benzene, hexabromo- (6CI,7CI,8CI,9CI); AFR 1001; FR-B; HBB; HBB (flame retardant); HBB-S; NSC 113975; Perbromobenzene; Plasafety HBB.

Human exposure: Hexabromobenzene (HBB) have been detected in human adipose tissues in Japan at a range of 2.1-4.1 ng/g wet wt, whereby pentabromobenzene and 1,2,4,5-Tetrabromobenzene seemed to be the major metabolites of HBB (Yamaguchi et al., 1988a).

Toxicity: Lowest toxic dose (TDLo) reported for HBB shown for rat for an intraperitoneal route of exposure was 150 mg/kg body wt giving biochemical effects on liver and porfyrin including bile pigments. For a continuous oral exposure to rat the TDLo were 3024 mg/kg/12weeks giving effects on liver, enzyme inhibition, induction, or change in blood or tissue levels and on esterases. Another study gave a TDLo for oral exposure on rat of 225 mg/kg/3days giving biochemical effects on liver, such as the activation of the hepatic microsomal mixed oxidases (RTECS, 2008). HBB was administered to mice as a single intraperitoneal dose of 20-90% of

the approximate lethal dose or acute intoxication. No histopatological changes where observed, but HBB decreased the liver glutathione (GSH) levels, increased the gamma-glutamyltrasferase activity in serum and increased the malondialdehyde in liver (Szymanska et al., 1998). The lowest toxic dose reported in birds for an oral exposure on quail and chicken was 1.5 g/kg/15 days and 52.5 g/kg/12 weeks, respectively. Toxic effects on quail were on liver, metabolic effects, enzyme inhibition, induction, or change in blood or tissue levels and porfyrin including bile pigments. Effects on chicken was effects on liver weight, weight loss or lack of weight gain, enzyme inhibition, induction, or change in blood or tissue levels and activation of hepatic mixed oxidase (RTECS, 2008).

Many studies on the effect of HBB on the heme synthesis in rat show HBB as a porfyrinogen (Mendoza et al., 1979;Smith and Francis, 1980;Koss et al., 1986;Szymanska and Piotrowski, 2000;Szymanska et al., 2002). Szymanska and Piotrowski concluded that based on these and previous results HBB should be classified as a porfyrinogen (Szymanska and Piotrowski, 2000). No teratogenic effects were observed for HBB when orally administered to rats during day 5 to 15 of gestation at the maximum concentration of 200 mg/kg (Khera and Villeneuve, 1975).

Placental transfer of HBB has been observed in rats and HBB is accumulated primarily in the adipose tissue (Villeneuve and Khera, 1975). For preweaning rat pups feeded by HBB treated dams, transmission through the milk had effect on pup liver weight but showed no effect on weight on other organs (Mendoza et al., 1978).

Eye/skin irritation: No data available.

Genotoxicity: HBB was tested for mutagenicity in the Salmonella/microsome preincubation assay using a protocol approved by the National Toxicology Program. A wide range of doses (10-10,000 μg/plate) was tested in four Salmonella typhimurium strains (TA98, TA100, TA1535, and TA1537) in the presence and absence of Aroclorinduced rat or hamster liver S9. These tests were negative (Haworth et al.,).

Endocrine effects: The ability of HBB to bind the AhR receptor and stimulate AhR transformation to its DNA binding form the gel retardation experiment and the CALUX bioassay was used. Results showed that HBB activate at a high concentration the AhR dependent gene expression at a similar concentration as decaBDE (Brown et al., 2004). Activation of selected cytochromes (CYP 1A and 2B) where shown in liver from rats administered intragastrically with HBB at 375 mg/kg/day for 7-28 days (Bruchajzer et al., 2004). 1,2,4,5-tetrabromobenzene was detected as a metabolite of HBB, and it was concluded that HBB and tetrabromobenzene are inductors of the microsomal enzyme system (Franklin et al., 1983;Bruchajzer et al., 2004). Effect of HBB and its metabolites on the level of glutathione peroxidase and transferase where studied in female Wistar rats. The rats was administered HBB intragastrically at 15, 75 and 375 mg/kg body wt. They concluded that HBB and the other studied BFRs increase the glutathione peroxidase and glutathione S peroxidase activity but only in the initial phase of

the experiment (Frydrych et al., 2005). HBB did not function as an agonist or antagonist (against dihydrotestosterone) on the androgen receptor in human hepatocellular liver carcinoma cells and did not successful interact with the ligand pocket (Larsson et al., 2006).

Absorption, distribution and excretion: 15 mg of HBB was administered to rat through a stomach tube during 4 months. Results showed a rapid elimination half-life of 2.5 days after treatment. The HBB concentrations were highest in the adipose tissue. (Koss et al., 1986). Metabolic fate was also studied on female rats, orally administered 16.6 mg/kg every other day for 2 weeks. Unchanged HBB and pentabromobenzene and O and S-containing metabolites were detected. HBB and metabolites were excreted in the ratio of 1 to 4 which suggests a high uptake rate and a high level of metabolization (Koss et al., 1982). Another study where HBB was orally administered to rats and tissue distribution and excretion was monitored showed half-lives for Phase I of 0.7 days and Phase II of 48 days, HBB seemed to be metabolized rapidly compared to HCB by reductive metabolization in the liver and was primarily excreted through feces (Yamaguchi et al., 1986;Yamaguchi et al., 1988b). In a study, ^{14}C labeled HBB was administered orally at doses of 600 mg/kg and 4500 mg/kg to female Wistar rats. The rats were monitored for 72 hours. Uptake rate (half-life phase I) was 1.2h and elimination half-life (phase II) was 440 hours. HBB accumulated primarily in the adipose tissue. Feces were the main route of excretion (75%) of the ^{14}C, 70% consisted of metabolites (and lower brominated bromobenzenes) (Sapota et al., 1997). HBB was assessed on uptake and elimination after dietary uptake in earthworms (*Eisenia Andrei*). Results indicate that HBB has a low uptake efficiency and biomagnification with an uptake efficiency between 0.7-7.5% and a BMF below 0.17 (Belfroid et al., 1993).

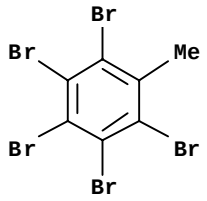
Bioaccumulation, degradation and fate: The bioconcentration and uptake rates, using perfused gills of Rainbow trout showed that HBB had similar uptake rate constant as hexachlorobenzene while it did not accumulate in Guppy (Sijm et al., 1993;Sijm et al., 1995). In another study the bioconcentration factor was determined for Rainbow trout, results was a BCF of 1100 which is a high bioconcentration factor (Oliver and Niimi, 1985) and an absorbtion efficiency of 0.28-0.18 while the whole body halflife was >13-31 days (Niimi and Oliver, 1988). Another laboratory study showed that HBB did not bioconcentrate or accumulate either from water or food by juvenile Atlantic salmon (Zitko and Hutzinger, 1976;Zitko, 1977).
An assessment of HBB fate has been done using a multimedia mass balance model (Fugacity model level III) and experimentally determined physico-chemical parameters. HBB is predicted to primarily distribute to soil (93%) and sediments (6.7%) and not to air and water (below 0.04%) (Kawamoto and Kuramochi, 2007). Tittlemier et al. (Tittlemier et al., 2002) also predicted HBB to be primarily distributed in soils (>98%) and sediments and the release into the environment would result in localized distributions.

Environmental levels: HBB was analyzed in pooled Herring gull egg samples from the Great Lakes of North America in 2004. Although present at

much lower levels than the PBDEs (0.24 – 0.53 ng/g wet wt), HBB was generally the most abundant of the non-PBDE BFRs. The authors concluded that there are non-PBDE BFRs in the aquatic food web of the Great Lakes (Gauthier et al., 2007). HBB has been detected in air (Gauthier et al., 2007) and sediments (Watanabe et al., 1986).

Emissions and monitoring data from the Nordic countries: In a screening for halogenated compounds in samples from an aluminum recycling plant, handling waste from electronics and electronics plastics and a car shredder, HBB was observed in all scrap samples (Sinkkonen et al., 2004). Further, HBB has been found in eggs and plasma of glaucous gulls in the Norwegian Arctic. Levels in egg yolk samples (0.4-2.6 ng/g wet wt) were comparable to those of the minor PBDEs (28, 116 and 155). Non-PBDE BFRs constituted only a small fraction of the total BFR content in egg yolk samples (Verreault et al., 2007).

4.1.2.2 Pentabromotoluene



Characteristics of the compound:

CAS No.:	87-83-2
CA Index name:	Benzene, 1,2,3,4,5-pentabromo-6-methyl-
Molecular Formula:	C7 H3 Br5
Molecular Weight (g/mol)	486.62[a]
Melting Point/range (°C)	280-282[b], 288[c], 299[c]
Boiling Point/range (°C)	394.4±37.0 [a]
Vapour Pressure (Pa (25°C))	1.22E-03[a]
Water Solubility (g/l (25°C))	7.80E-04 [a]
Partition Coefficient (log P_{ow})	5.872±0.615 [a], 5.43[c]
Partition Coefficient (log K_{oc})	4.57 [a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04).
b) Data from the SciFinder data base originating from experimentally determined properties.
c) Data from a report by the Danish EPA (Simonsen et al., 2000).

Known uses: Used in the formulation of glass reinforced unsaturated polyester compounds used in electrical applications as flame retardant in bulk moulding compounds (OECD, 1994).

Synonyms: Benzene, pentabromomethyl- (9CI); Toluene, 2,3,4,5,6-pentabromo- (6CI,7CI,8CI); 1,2,3,4,5-Pentabromo-6-methylbenzene; 2,3,4,5,6-Pentabromomethylbenzene; 2,3,4,5,6-Pentabromotoluene; Flammex 5BT; PBT; PBT (flame retardant); Pentabromomethylbenzene.

Human Exposure: No data available.

Toxicity: Sprague-Dawley rats (15 rats/sex/dose level) were exposed to pentabromotoluene (PBT) in the diet 0.05 to 500.0 mg/kg diet (≈ 0.003-40 mg/kg body wt/day) for 91 days. No clinical signs of toxicity were observed, and growth rate and food consumption was not affected. PBT caused no dramatic changes in biochemistry, haematology and gross pathology. Mild dose-dependent histological changes were observed in the thyroid, liver, and kidney of rats fed PBT diets. The no observed adverse effect level (NOAEL) was 5.0 mg/kg diet (≈ 0.35 mg/kg body wt/day) (Chu et al., 1987). PBT was administered to rat and the TDLo was 4200 mg/kg/28days and 13.65 g/kg/91days with effects on liver and kidney/ureter/bladder and endocrine effects such as changes in tyroid weight and effect on haematology (normocytic anemia) (RTECS, 2008). The LC_{50} for

fish was > 5 mg/l (48 hours) (Simonsen et al., 2000). No adverse foetal effects were observed when doses up to 600 mg/kg body wt were given orally to rats during organogenesis (Simonsen et al., 2000).

Eye/skin irritation: No data available.

Genotoxicity: PBT was tested for mutagenicity in the Salmonella/ microsome preincubation assay using a protocol approved by the National Toxicology Program. A wide range of doses (100 - 10,000 μg/plate) was tested in four Salmonella typhimurium strains (TA98, TA100, TA1535, and TA1537) in the presence and absence of Aroclorinduced rat or hamster liver S9. These tests were negative and the highest ineffective dose level tested (not causing the formation of a precipitate) in any Salmonella tester strain was 100 μg/plate (Zeiger et al., 1987).

Endocrine effects: Examination of receptor binding and activation by BFRs through the Ah receptor reporter gene assay demonstrated the ability of pentabromotoluene to bind to the Ah receptor to levels comparable to 2,3,7,8-tetrabromodibenzodioxin (TCDD). Results also showed that this compound were able to stimulate AhR dependent gene expression at high concentrations, but was significantly less potent than the flame retardant PHT4 (primary constituent: Tetrabromophthalic anhydride) and decaBDE. Further, it was three orders of magnitude less potent than TCDD (Brown et al., 2004).

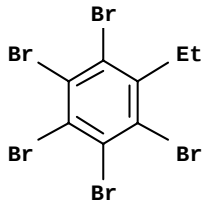
Absorption, distribution and excretion: No data available.

Bioaccumulation, degradation and fate: Studies of dietary absorption efficiency in rainbow trout and BCF showed that PBT had an absorption efficiency of 0.18-0.28 and whole-body half-life of 13-23 days and a BCF of 270 (Oliver and Niimi, 1985;Niimi and Oliver, 1988). The bioconcentration factor in fish was determined to 4.5-39 (Simonsen et al., 2000). PBT was found to not be readily biodegradable (7% of BOD, 4weeks, 100 mg/l substance, 30 mg/l sludge) (Simonsen et al., 2000).

Environmental levels: Pentabromotoluene was analyzed in egg pools of Herring gull from the Great Lakes of North America in 2004. Results showed much lower levels than for PBDEs (0.004 – 0.02 ng/g wet wt) and were generally the lowest of the non-PBDE BFRs. The authors concluded that the results suggests that there are non-PBDE BFRs in the aquatic food web of the Great Lakes (Gauthier et al., 2007).
In a screening of sediment samples from the Elbe river and its tributaries for new contaminants, pentabromotoluene showed a concentration range of <1-25 ng/g dry wt (Schwarzbauer et al., 2001).

Emissions and monitoring data in the Nordic countries: Sewage sludge samples from Swedish waste-water treatments plants contained a few brominated toluenes such as penta- and two isomers of tetra-bromotoluene (Mattsson et al., 1975).
PBT have been found in eggs and plasma from glaucous gulls in the Norwegian arctic. Levels in plasma was in the range of <LOQ-0.15 ng/g wet wt and egg yolk samples <LOQ-0.12 ng/g wet wt (Verreault et al., 2007).

4.1.2.3 Pentabromoethylbenzene



Characteristics of the compound:

CAS No.:	85-22-3
CA Index name:	Benzene, 1,2,3,4,5-pentabromo-6-ethyl-
Molecular Formula:	C8 H5 Br5
Molecular Weight (g/mol)	500.65[a]
Melting Point/range (°C)	138[b]
Boiling Point/range (°C)	413.3±40.0[a]
Vapour Pressure (Pa (25°C))	3.2E-04[a]
Water Solubility (g/l (25°C))	3.50E-04[a]
Partition Coefficient (log P_{ow})	6.403±0.615[a]
Partition Coefficient (log K_{oc})	4.86[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04).
b) Data from the SciFinder data base originating from experimentally determined properties.

Known uses: Flame retardant for textiles, adhesives and polyurethane foam. Thermoset polyester resins, coatings. Additive for unsaturated polyesters (WHO, 1997).

Synonyms: Benzene, pentabromoethyl- (6CI,7CI,8CI,9CI); 2,3,4,5,6-Pentabromo-ethylbenzene; EB 80; Hexel.

Human Exposure: No data available.

Toxicity: Administration of pentabromoethylbenzene (PBEB) onto the skin of rabbit's gave an LD_{50} > 8g/kg, no details was reported on effects (RTECS, 2008).

Eye/skin irritation: No data available.

Genotoxicity: Pentabromoethylbenzene (PBEB) was tested for mutagenicity in the Salmonella/microsome preincubation assay using a protocol approved by the National Toxicology Program. A wide range of doses (333-10,000 µg/plate) was tested in four Salmonella typhimurium strains (TA98, TA100, TA1535, and TA1537) in the presence and absence of Aroclor-induced rat or hamster liver S9. These tests were negative (Zeiger et al., 1987).

Endocrine effects: No data available.

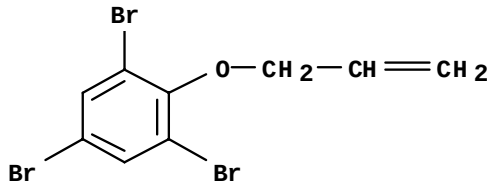
Absorption, distribution and excretion: No data available.

Bioaccumulation, degradation and fate: Studies of dietary absorption efficiency in rainbow trout and BCF showed that PBEB had an absorption efficiency of 0.26 and whole-body half-life of 38 days while the bioconcentration study resulted in a moderate BCF of 330 (Oliver and Niimi, 1985;Niimi and Oliver, 1988).

Environmental levels: PBEB was analyzed in egg pools of Herring gull from the Great Lakes of North America in 2004. PBEB levels were found in the range of 0.03 – 1.4 ng/g wet wt, which is 0.7 % compared to sum PBDEs (47, 99, and 100) (Gauthier et al., 2007). A study by Hoh et al. reported a relatively high abundance of PBEB in the atmosphere of Chicago (summer of 2003). PBEB was detected in both gas and particle phases (520 pg/m^3 gas phase and 29 pg/m^3 in particle phase), with peak intensities 100 times higher than for the PBDEs (sum PBDEs tri-hexa of 47 pg/m^3). Other compounds such as tetrabromoethylbenzenes, which the authors believe to be byproducts of PBEB, were detected but not quantified (Hoh et al., 2005). Screening of air samples in three locations in UK and Ireland (reference site) reported a mean concentration of PBEB of 30 pg/m^3 in the southwest Oxford (Lee et al., 2002).

Emissions and monitoring data in the Nordic countries: Filter dust, cyclone dust and light fluff samples of an aluminium recycling plant in Finland, handling waste from electronics and electronics plastics and a car shredder was screened for halogenated compounds. PBEB was observed in all scrap samples with quite high concentrations (no concentrations was assigned), and was among the most abundant alkylbromobenzenes (Sinkkonen et al., 2004). PBEB have been found in eggs and plasma from glaucous gulls in the Norwegian arctic. PBEB was below the method limit of quantification (MLOQ) values in plasma and was only detected in the range (0.03-0.23 ng/g wet wt) in egg yolk samples. Non-PBDE BFRs constitute only a small fraction of the total BFR content in egg yolk samples (Verreault et al., 2007).

4.1.2.4 2,4,6-Tribromophenyl allyl ether



Characteristics of the compound:

CAS No.:	3278-89-5
CA Index name:	Benzene, 1,3,5-tribromo-2-(2-propen-1-yloxy)-
Molecular Formula:	C9 H7 Br3 O
Molecular Weight (g/mol)	370.86[a]
Melting Point/range (°C)	Not available
Boiling Point/range (°C)	339.5±37.0[a]
Vapour Pressure (Pa (25°C))	4.9E-02[a]
Water Solubility (g/l (25°C))	2.0E-02[a]
Partition Coefficient (log P_{ow})	4.974±0.564[a]
Partition Coefficient (log K_{oc})	4.08[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04).

Known uses: Flame retardant used in Expandable polystyrene (EPS) (WHO, 1997).

Synonyms: Benzene, 1,3,5-tribromo-2-(2-propenyloxy)- (9CI); Ether, allyl 2,4,6-tribromophenyl (7CI,8CI); 2,4,6-Tribromophenyl allyl ether; Allyl 2,4,6-tribromophenyl ether; NSC 35767; Pyro-guard FR 100; bromkal 64-3AE; Great Lakes PHE-65.

Human Exposure: No data available.

Toxicity: No data available**.**

Eye/skin irritation: No data available.

Genotoxicity: No data available.

Endocrine effects: No data available.

Absorption, distribution and excretion: No data available.

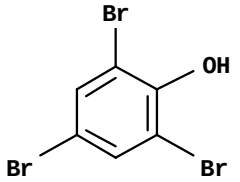
Bioaccumulation, degradation and fate: 2,4,6-Tribromophenyl allyl ether (ATE) was proposed to be one of 120 high production chemicals which are structurally similar to known arctic contaminants and/or have partitioning properties that suggests they are potential arctic contaminants (Brown and Wania, 2008).

Environmental levels: ATE was found in blubber and brain of hooded and harp seal from the Barents sea at concentrations of 5.4 – 9.1 and 3.1 – 10 ng/g wet wt, respectively (Vetter, 2001;Von Recke and Vetter, 2007). The authors

showed that an experimental aerobic degradation using corrinoids reduced 2,3-dibromopropyl-2,4,6-tribromophenyl ether (DPTE), which is the main component of Bromkal 73-5 PE, to ATE and 2-bromoallyl-2,4,6-tribromophenyl ether. Comparing the ratio in blubber and brain in harp seal showed that DPTE is the more prominent BFR in these samples (ratio ATE/DPTE of 0.018 in blubber and 0.030 in brain) and the authors conclude that the presence of ATE is probably mainly due to the transformation of DPTE (Von Recke and Vetter, 2007). ATE have also been detected in 15 of 18 municipal sewage sludge samples in Germany from 10 different sewage treatment plants at a range of < 0.005-0.091 mg/kg dry wt. Also DPTE was found in 12 out of 18 samples at a range of < 0.025-0.596 mg/kg dry wt (ratio of the mean ATE/DPTE of 0.17) proving that ATE and DPTE is not degraded in these sludge treatment processes (Weisser, 1992). These types of compounds seems also to accumulate to a higher degree than PBDEs in brain tissues of harp seal and seems to pass the blood-brain barrier (Von Recke and Vetter, 2007).

Emissions and monitoring data in the Nordic countries: No data available.

4.1.2.5 2,4,6-tribromophenol



Characteristics of the compound:

CAS No.:	118-79-6
CA Index name:	Phenol, 2,4,6-tribromo-
Molecular Formula:	C6 H3 Br3 O
Molecular Weight (g/mol)	330.80[a]
Melting Point/range (°C)	94-95[b], 95-96[b], 95.5[c], 87-89[c]
Boiling Point/range (°C)	286.8[b], 244[c], 282-290[c]
286[c]Vapour Pressure (Pa (25°C))	0.41[a]
Water Solubility (g/l)	1.30[b], 7.1E-2 (at 15°C)[c]
	0.995 (at 15°C)[c]
	0.968 (at 25°C)[c]
	0.883 (at 35°C)[c]
Partition Coefficient (log P_{ow})	4.326±0.486[a], 4.02[c], 3.3[c]
Partition Coefficient (log K_{oc})	2.98 (pH 7)[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Data from SciFinder data base originating from experimentally determined properties
c) Data from a report by the Danish EPA (Simonsen et al., 2000)

Known uses: Antiseptic and germicide in e.g., pharmaceutical preparations. Flame retardant in thermoplastic polyester and epoxy resins, in acrylonitrile-butadiene-styrene resins, in phenolic resins and polystyrene. Chemical intermediate for its bismuth salt (antiseptic), for pentachlorophenol and for 2,4,6-tribromophenoxy compounds (Simonsen et al., 2000). 2,4,6-tribromophenol (TBP) also have been used as a fungicide for wood presservation (Nichkova et al., 2008).

Synonyms: 1,3,5-Tribromo-2-hydroxybenzene; Bromkal Pur 3; Bromol; Flammex 3BP; NSC 2136; PH 73.

Human Exposure: NIOSH (NOES Survey 1981-1983) has statistically estimated that 1427 workers (734 of these are female) are potentially exposed to TBP in the US. Occupational exposure to 2,4,6-tribromophenol (TBP) may occur through inhalation and dermal contact with this compound at workplaces where TBP is produced or used. Monitoring data indicate that the general population may be exposed to TBP via ingestion of food and drinking water, and by dermal contact with this compound (TOXNET, 2008). TBP have been found in young Nicaraguan women with an indication that environmental exposure due to their living close to

waste disposal sites increases TBP levels (Cuadra et al., 2003).

Toxicity: Oral LD_{50} values during an administration of TBP to male and female rats was 1,995 and 1,819 mg/kg body wt, respectively (Simonsen et al., 2000). Another study on male and female rats resulted in oral LD_{50} values of 5,012 and 5,012 mg/kg body wt, respectively. Signs of toxicity included decreased motor activity, nasal discharge, lacrimation, tremors, prostration, clonic convulsions and death (Simonsen et al., 2000).

Inhalation studies on rat showed an LC_{50} >1630 mg/m^3/4 hours, with effects on sense organs (ptosis on eye) (RTECS, 2008). An inhalation study of dust with TBP gave an LC_{50} of >1.63 mg/l/4 hours (65% of the particles were less than 6 microns) and another study with an LC_{50} of >200 mg/l/1 hour tested at two concentration levels 2 or 200 mg/l. Signs at both concentrations included nasal discharge, eye squint, increased followed by decreased respiratory rates, prostration, salivation, lacrimation, erythema, increased followed by decreased motor activity, and ocular and nasal porphyrin discharge. No details were available about f.ex. particle size or distribution. All rats appeared normal from day 7 post exposure, except on day 10 of the 14 day observation period when one rat at low exposure level exhibited nasal porphyrin discharge (Simonsen et al., 2000).

Dermal administration of TBP on rabbit gave an LD_{50} of >2000 mg/kg body wt and >8,000 mg/kg body wt (Simonsen et al., 2000). Three groups of rats each consisting of 5 males and 5 females in a subchronic toxicity study, were exposed (whole-body) to atmospheric dust concentrations (analytical) of 0, 0.10 and 0.92 mg/l, respectively, for 6 hours/day, 5days/week, for 3 weeks. The NOAEL in this study appears to be <0.10 mg/l for females and 0.10 mg/l for males. No dermal toxicity to albino rabbits during a 28-day sub acute dermal toxicity study was observed (Simonsen et al., 2000).

TBP inhalation of 100 µg/m^3/24 hours for female rats during 1-21 days after conception gave fetotoxicity (except death, eg. stunted fetus), developmental abnormalities and behavioral changes of the newborn pup. TBP inhalation study on female mouse of 0.15mg/m^3, 122 days pre-mating, showed post implantation mortality and fetotoxicity (RTECS, 2008).

In a pilot study, mated Charles River CD female rats were dosed with TBP by gavage at 10 to 3,000 mg/kg/day from gestation day 6 through day 15. All animals died at the highest dose group after one day of treatment. There were slight decreases in body weight gains between days 6 and 12, an increase in post implantation losses, and a slight decrease in the number of viable foetuses at the 1,000 mg/kg/day dose group. The NOAEL appears to have been 300 mg/kg/day for both dams and fetuses (embryotoxicity). In order to investigate the developmental neurotoxicity and immunotoxicity, pregnant Wistar rats were exposed to TBP by inhalation 0.03 - 1.0 mg/m^3, from day 1 to 21 of gestation. The results suggested that TBP during this exposure regime may be a developmental neurotoxicant, embryotoxicant and foetotoxicant but not immunotoxicant. The NOAEL for developmental neurotoxicity could not be established (<0.03 mg/m^3), and the

NOAEL for maternal neurotoxicity was 0.3 mg/m^3 (Simonsen et al., 2000).

Pregnant wistar rats were orally administered Aroclor 1254, hydroxylated PCBs, BDE-47 and TBP (25mg/kg/day) during gestational day 10-16. They monitored endocrine effects, developmental landmarks, sexual and neurobehavioural development and transplacental transfer. Results indicated that the hydroxylated PCB metabolites and BFRs are capable of placental transfer while no effects was observed (at these concentrations) on the developmental landmarks (Buitenhuis et al., 2004).

For tribromophenol the LC_{50} (in fish) was 6.5-6.8 mg/l (96 hours, fathead minnow) and 1.1 mg/l (96 hours, fathead minnow, flow through bioassay) (Simonsen et al., 2000).

Eye/skin irritation data: TBP is not an skin irritant but a mild eye irritant when administering into the eye of 100 mg using the standard draize test on rabbit (RTECS, 2008). TBP was shown to be irritating to the respiratory tract and gives irritation to mucous membranes and skin sensitisation agent in Guinea pigs (Simonsen et al., 2000).

Genotoxicity: TBP was tested for mutagenicity in *Salmonella typhimurium* strains TA98, TA100, TA1535, TA1537 and TA1538, and in *Saccharomyces cerevisiae* strain D4 in the presence and absence of metabolic activation. TBP was negative in all test assays (Simonsen et al., 2000).

Endocrine effects: The steroidogenic enzyme aromatase (CYP 19) was studied on in vitro H295R human adrenocortical carcinoma cells. Results demonstrated that TBP had a concentration dependent induction of aromatase activity at levels of 0.5 to 7.5 μM (Canton et al., 2005).

Absorption, distribution and excretion: A single oral dose of ^{14}C-labeled TBP (4.0-5.3 mg/kg body wt) was rapidly absorbed in rats. 48 hours after the administration, 77% of the radioactivity was excreted via the urine and 2-14% via faeces, and detectable radioactivity was measured in kidneys, lungs and liver. Blood concentrations peaked 1 hour after dosing at 4.57 ppm and then plunged to 0.002 ppm by 24 hours (half-life in blood: 2.03 hours). The pharmacokinetics appeared to follow a one-compartment open model. TBP was rapidly distributed in the body, and the elimination in the urine was proportional to the concentration in the blood (Simonsen et al., 2000).

Bioaccumulation, degradation and fate: Aerobic biodegradation was tested using TBP at 100 mg/l in an activated sludge inoculum in the Japanese MITI test. It reached 49% of its theoretical BOD in 28 days. TBP was not degraded over 14 days in a marine sediment slurry. No ring degradation was reported for TBP at 100 mg/l, over a 5-day period using a soil inoculum. Water samples collected from two treatment ponds were unable to degrade TBP over 32 days (TOXNET, 2008). An anaerobic degradation test showed that TBP was rapidly dehalogenated with >90% degradation in 2 days in a marine sediment slurry. A first-order rate constant of 0.19 day^{-1} was reported for TBP in anoxic sediment from Loosdrechtse Plassen (TOXNET, 2008). BCF values of 513 and 83 were measured in zebrafish and fathead minnow, respectively,

for TBP. These BCF values suggest that the potential for bioconcentration in aquatic organisms is moderate to high (Simonsen et al., 2000). Flodin et al. studied the biosynthesis pathway of bromophenols from the green marine algae *Ulva lactuca* showing that certain precursors are converted to bromophenols by the bromoperoxidase (Flodin and Whitfield, 1999). As the ecological function of bromophenols are not yet clear, researchers suggests that they may play a role as a natural chemical defense and deterrence (Hassenkloever et al., 2006).

TBP was proposed to be one of 120 high production chemicals which are structurally similar to known arctic contaminants and/or have partitioning properties that suggests they are potential arctic contaminants (Brown and Wania, 2008).

Risk assessment: TBP has been evaluated and results were retrieved through the Hazardous Substances Data Bank (HSDB) (TOXNET, 2008). Results from the assessment suggested that the current use of TBP as a flame retardant, a flame retardant intermediate and a wood preservative may result in its release to the environment through various waste streams. Based on the estimated vapor pressure of 0.082 Pa at 25 °C they suggested that TBP will exist in both the vapor and particulate phases in the ambient atmosphere with an estimated half-life in air of 34 days. Parti-culate-phase TBP will be removed from the atmosphere by wet and dry depo-sition. If released to soil, TBP is expected to have slight mobility based upon an estimated Koc of 4200. An estimated pKa of 6.0, indicates that TBP can exist as an anion in the environment. Anions generally do not adsorb to organic carbon and clay more strongly than their neutral counterparts. Volatilization from moist soil surfaces of non-dissociated TBP is not expected to be an important fate process based upon an estimated Henry's Law constant of $3.6x10^{-8}$ atm-m^3/mole. The anion is also not expected to volatilize from soil surfaces. No data were located reporting the aerobic biodegradation of TBP in soil; however, biodegradation in aerobic marine sediment did not occur over a 14 day period. If released into water, TBP is expected to adsorb to suspended
solids and sediment based upon the estimated Koc. While this compound is resistant to aerobic biodegradation, dehalogenation in anaerobic sediments should occur rapidly, with a reported half-life of approximately 4 days. This compound's pKa indicates that TBP will exist almost entirely in the ionized form at pH values of 5 to 9 and therefore, volatilization from water surfaces of the anion is not expected to be an important fate process. Volatilization from water surfaces of non-dissociated TBP is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. Bioconcentration in aquatic organisms is suggested to be moderate to high. Occupational exposure to TBP may occur through inhalation and dermal contact with this compound at workplaces where TBP is produced or used. Monitoring data indicate that the general population may be exposed to TBP via ingestion of food and drinking water, and dermal contact with this compound and other products containing TBP (TOXNET, 2008). Also, an environmental assessment made by the Danish EPA suggests an LC50 between 1 mg/l and 10mg/l and a log $P_{OW} > 3$ (in its protonated state) and the substance not being readily biodegrade-

able indicate that TBP may be considered to be toxic to aquatic organisms and may also be able to cause long-term adverse effects in the aquatic environment (Simonsen et al., 2000).

Health assessment: Conclusions drawn from an health assessment study by the Danish EPA (Simonsen et al., 2000) of 2,4,6-tribromophenol showed that sufficient toxicological data were available to make a health assessment, even if there is a lack of data such as, eg. chronic toxicity, carcinogenicity or reproductive toxicity and no data on humans were identified. They concluded that TBP seems to be only slightly acute toxic after oral, dermal or inhalation exposure. TBP is slightly skin irritating and moderately eye irritating. Based on a preliminary test, it may have a skin sensitizing potential. TBP was not mutagenic when tested in an *in vitro* gene mutation tests. The tests for subchronic inhalation and dermal toxic-ity did not reveal any indications of possible danger or risks of irreversible health effects by prolonged exposure. A preliminary study indicated that TBP might be embryotoxic at oral dosage levels causing only a slight decrease in maternal weight gain during the gestational exposure period. Inhalation of TBP may cause specific developmental neurotoxicity, embryotoxicity and foetotoxicity (Simonsen et al., 2000).

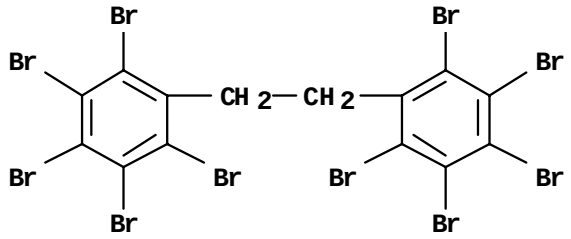
Environmental levels: Endeavour prawns from Exmouth Gulf, Shark Bay, and Groote Elylandt, Australia, contained TBP at concentrations of 41 to 97, 7.8, and 8.5 ug/kg, respectively (Whitfield et al., 1992). Ten different species of fish, collected in August 1992 from the eastern coast of Australia, contained TBP at concentrations of <0.05 to 3.4 ng/g for the carcass and <0.05 to 170 ng/g for the whole gut (analysis of single fish from each species) (Whitfield et al., 1995). Ocean fish were separated by species into pelagic carnivores, benthic carnivores, diverse omnivores and restricted omnivores; concentrations in the flesh ranged from <0.01 to 0.9 ng/g, <0.01 to 12 ng/g, <0.01 to 4.3 ng/g, and 0.1 to 1.4 ng/g, respectively, while concentrations in the gut ranged from <0.01 to 11 ng/g, <0.01 to 230 ng/g, 0.04 to 55 ng/g, and 7 to 45 ng/g, respectively (Whitfield et al., 1998). Marine fish (Salmon), crustaceans and mollusks from the Pacific Ocean contained bromophenols while only low levels was found in freshwater salmon from the Great Lakes (Boyle et al., 1992).
Thirty samples of 9 species of prawns, collected from the eastern coast of Australia from 1993 to 1996, contained TBP at concentrations of <0.01 to 170 ng/g while TBP concentrations in cultivated prawns ranged from <0.01 to 0.53 ng/g (Whitfield et al., 1997). Concentrations of TBP were measured in brown algae (14 to 38 ug/kg wet weight), red algae (4.5 to 68 ug/kg), bryozoa (24 and 27 ug/kg), a hydroid (29 ug/kg), and sponges (0.22 to 240 ug/kg) collected from Exmouth Gulf, Australia, in October 1990 (Whitfield et al., 1992). An analysis of selected Hong Kong seafood (eg. rabbitfish, clam and shrimp) as well as brown algae found concentrations of the total bromophenol content to be 40-7000 ng/g dry wt, which varied with the season with crab having the highest seasonal concentration of mono- di- and tribromophenols (Chung et al., 2003a;Chung et al., 2003b). Ahn et al. found sponges to contain brominated organic compounds up to 12% of the dry wt of eg. bromoindoles, bromophenols

(mono-, di- and tribromophenol), and bromopyrroles and showed that these aerophobic sponges harbor bacteria that are capable of an reductive dehalogenation processes (Ahn et al., 2003). Upper river and marine sediment layers in Osaka Prefecture, Japan, collected in 1981 through 1983 at 12 different locations, contained TBP at concentrations ranging from <0.2 ppb to 35 ug/kg dry wt (Watanabe et al., 1985). Surficial sediments from 5 sampling sites in the Rhone estuary, collected in 1987/1988, contained TBP at concentrations of 26 to 3690 ng/g dry wt (Tolosa et al., 1991).
TBP have been found in wine as contaminants from old winerys originating from structural elements of the winery or the wooden containers (Chatonnet et al., 2004). TBP might be found as a product in the combustion of tribromoaniline and SB_2O_3 flame retarded materials such as textiles and plastics (Bindra and Narang, 1995). Indoor dust in Japan was studied for potential thyroid disrupting compounds suggesting that TBP and pentachlorophenol are potential thyroid disrupting compounds in homes and work environments of Japan and other counties while indoor dust also is an important exposure route to children (Suzuki et al., 2008).

Emissions and monitoring data in the Nordic countries: The raw flue gas from a Swedish hazardous waste incinerator, located at Norrtorp, and fed chlorinated (mainly solvents) and brominated waste (tetrabutylammonium bromide) contained TBP at <14, 380, and 260 ng/m^3 over three tests; bromides were present initially at 32, 110, and 530 mg/m^3. Flue gas from this incinerator, fed municipal waste, contained TBP at 4-5 ng/m^3. Peat combustion released TBP at concentrations of <5 to 60 ng/m^3 (Oeberg et al., 1987). TBP was analysed among other FRs (TBBP-A and PBDEs) in 22 municipal waste water treatment plants. TBP was in the range n.d. to 0.9 ng/g wet wt (Oberg et al., 2002). During an investigation of sediments and water in the North and Baltic sea, TBP was found in water samples from the the German Bight in the range of n.d. to 6 ng/l but not found in any of the investigated sediment samples (Reineke et al., 2006). A study on the occupational exposure to BFRs in Norwegian workers at an electronics dismantling plant, plasma samples was collected and analysed for PBDEs, halogenated phenols (including TBP) and tetrachloro- and bromobisphenol A. TBP was generally the most abundant BFR at 0.17 to 81 ng/g lipid wt (Thomsen et al., 2001). In a study on temporal trends (1977-2003) and the role of age, pooled serum samples from the Norwegian population was analysed for BFRs. TBP was found not to follow a similar trend as PBDEs. PBDEs increased from 0.5 ng/g lipid wt in 1977 to 4.8 ng/g lipid wt in 1988 and the levels stabilized from 1989 to 2003 while TBP showed no relations to trends or age which might be due to short half-lives of TBP in humans (Thomsen et al., 2002;Thomsen et al., 2007).

4.1.3 Polyaromatics

4.1.3.1 Decabromodiphenylethane



Characteristics of the compound:

CAS No.:	84852-53-9
CA Index name:	Benzene, 1,1'-(1,2-ethanediyl)bis[2,3,4,5,6-pentabromo-
Molecular Formula:	C14 H4 Br10
Molecular Weight (g/mol)	971.22[a]
Melting Point/range (°C)	334-337[b], 344-349[c] 348-353[d], 351-355[d]
Boiling Point/range (°C)	676+/-50[a]
Vapour Pressure (Pa (25°C))	6.0E-15[a], <1E-04 (20°C)[d]
Water Solubility (g/l (25°C))	2.10E-07[a], 7.2E-04[d]
Partition Coefficient (log P_{ow})	11.1[a]
Partition Coefficient (log K_{oc})	7.0[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Data from the SciFinder data base originating from experimentally determined properties
c) Experimental data from Li et al. (Li et al., 2004)
d) Experimental data from the UK EPA (Dungey and Akintoye, 2007)

Known uses: For use in HIPS. It can also be used in ABS, PC/ABS and HIPS/PPO polymers (Ecology, 2006). Decabromodiphenyl ethane (DBDPE) was introduced into the market as an alternative for DecaBDE (Kierkegaard et al., 2004).

Synonyms: 1,2-Bis(2,3,4,5,6-pentabromophenyl)ethane; 1,2-bis(pentabromophenyl)ethane; Decadiphenyl 8010; Ethylenebis (pentabromobiphenyl); Ethylenebispentabromobenzene; FCP 801; Fire-master 2100; Planelon BDE; S 8010; Saytex 8010.

Human Exposure: No evidence of skin sensitization properties was observed on 200 professional workers from Wei-Dong Chemical Company during a repeated application of DBDPE in petrolatum during three weeks (Li et al., 2004).

Toxicity: Single dose and long term (90 days) oral administration of DBDPE in rats resulted in high LD_{50} values (> 5000 mg/kg body wt) and LDLo (90 g/kg/90 days) where the highest doses gave changes in liver weight and slight histomorphological effects. The dermal

acute toxicity (LD_{50}) in rabbits was > 2000 mg/kg body wt, the NOAEL in rat was estimated to ≥1000 mg/kg/day (Hardy et al., 2002;RTECS, 2008) while the inhalation route is not suspected by the Canadian centre for occupation health and safety to be acutely toxic (RTECS, 2008). Authors conclude that the lack of toxicity for DBDPE is likely due to poor bioavailablity due to its high molecular weight and poor water solubility (Hardy et al., 2002). Acute toxicity data on ingestion, inhalation, dermal contact in rat at a maximum concentration of oral - 2000mg/kg body wt (single dose), dermal – 2000 mg/kg body wt (24 hours) and inhalation – 50 mg/l (1 hour). Results proved that DBDPE exhibit a low acute oral, dermal and inhalation toxicity (Li et al., 2004).

Eye/skin irritation: DBDPE is not suspected to be a skin or eye irritant (TOXNET, 2008).

Genotoxicity: Based on structurally similar analogues The EPA have determined that this material may cause cancer (TOXNET, 2008).

Endocrine effects: No data available.

Absorption, distribution and excretion: No data available.

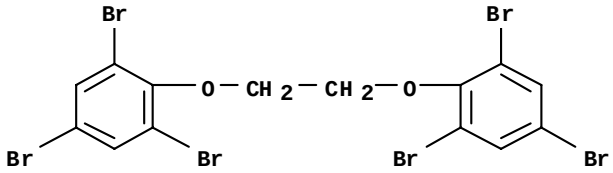
Bioaccumulation, degradation and fate: DBDPE was considered to be not redily biodegradable in an activated sludge inocculum, tested in compliance with the OECD test guidelines 301C (modified MITI test). 100 mg/l of DBDPE with a purity of 96.6 % was incubated with 30 mg/l activated sludge at 25°C over 28 days. No degradation was observed as measured by the BOD. The risk evaluation report by UK EPA suggested that DBDPE is unlikely to be rapidly degraded, based on biodegradation results, above, and calculations on the atmospheric (OH radical) and aquatic (hydrolysis) degradation rates. They stated that other degradation mechanisms cannot be excluded, such as anaerobic degradation as may be found in WWTP (Dungey and Akintoye, 2007).
DBDPE did not bioconcentrate (BCF of <2.5-<25) in Japanese carp during an 8 week exposure while compounds with an molecular weight below 700 Da did bioconcentrate (Hardy, 2004). Biomagnification was observed in between the trophic levels of Lake Winnipeg (Canada) food web resulting in an BMF of 0.2-9.2 for DBDPE, and was highest between the top predator Walleye and bottom-feeding white suckers with an BMF of 9.2 (Law et al., 2006;Law et al., 2007).

Environmental levels: A food web study of Lake Winnipeg (Canada) observed this compound for the first time in fish (Walleye) with the highest mean concentration of DBDPE of 1.0 ± 0.5 ng/g lipid wt while it was not detected in zooplankton, mussels, and whitefish. The concentration in sediments was below the method detection limit (MDL) and the concentration in lake water was difficult to measure due to the high lipophilicity of DBDPE (Law et al., 2006;Law et al., 2007). Several non-PBDE BFRs was detected in a study of egg pools of herring gulls (Larus argentatus) from seven colonies in the Great Lakes (collected in 1982 to 2006). The concentrations of DBDPE in eggs from 2005 and 2006 of three of the seven colonies were 1.3 to 288 ng/g wet wt and surpassed decaBDE. The authors concluded that there is an indication that

there have been a continual exposure and bioaccumulation of several BFRs in the Great Lakes (Gauthier et al., 2008).
DBDPE was recently detected in two species of captive panda in China in 87 and 71 % of the giant and red panda samples, at concentrations up to 863 ng/g lipid wt, respectively. DBDPE and decaBDE dominated the samples and the authors suggested that these levels might relate to significant production, use or disposal of BFRs in China (Hu et al., 2008).
DBDPE have been found in house dust in the U.S. ranging from <10 to 11070 ng/g dust wt with a median value of 201 ng/g dust wt (Stapleton et al., 2008), which is ten times higher than the levels found in Sweden (Karlsson et al., 2007).
DBDPE have also been found primarily in the particulate phase in air near the Great Lakes (U.S.) at median concentrations from 1 to 22 pg/m^3(Venier and Hites, 2008) and have been found in tree bark from the Northeastern U.S. ranging from ND to 0.73 ng/g bark wt (Qiu and Hites, 2008).

Emissions and monitoring data in the Nordic countries: BFRs were determined in air, sedimentary dust and plasma from five households in Sweden. DBDPE was not detected in plasma but in one of the five air samples at a concentration of 0.013 ng/m^3, while in sedimentary dust the DBDPE was among the most abundant BFRs with an average concentration of 47ng/g dust wt, 1/10 of the concentration of BDE-209. Due to the limited data no firm conclusions could be drawn on the relationship of the plasma and air or dust levels while sumBDE concentrations correlated between plasma and dust levels. The author suggests that as BTBPE and DBDPE were found in household dust at similar concentrations as many of the PBDEs, show that humans and especially toddlers are exposed to these compounds in their homes via the dust (Karlsson et al., 2007).
DBDPE was monitored in wastewater, sludge, sediment and indoor air in Sweden. DBDPE was observed in 25 of 50 Swedish waste water treatment facilities with an estimated concentration of 100 ng/g dry wt, an air sample from an electronic dismantling plant showed a concentration of 0.6 ng/m^3 and DBDPE was also found in water piping insulation (Kierkegaard et al., 2004).
To evaluate exposure to BFR in an electronic recycling facility, personal air monitoring was done for 2 years. A total of 22 polybrominated di-Ph ethers (PBDE) and 2 other Br-containing organic compounds were analyzed and evaluated in 17 personal air samples (Pettersson-Julander et al., 2004). One of the compounds was identified as as 1,2-bis(2,4,6-tribromophenoxy)ethane (BTBPE) based on full scan spectra and previous identifications (Sjodin et al., 2001), the other compound was tentatively identified as DBDPE based on fullscan spectra (Pettersson-Julander et al., 2004).

4.1.3.2 1,2-bis(2,4,6-tribromophenoxy)ethane



Characteristics of the compound:

CAS No.:	37853-59-1
CA Index name:	Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis[2,4,6-tribromo-
Molecular Formula:	C14 H8 Br6 O2
Molecular Weight (g/mol)	687.64[a]
Melting Point/range (°C)	Not available
Boiling Point/range (°C)	566.4±50.0[a]
Vapour Pressure (Pa (25°C))	3.88E-10[a]
Water Solubility (g/l (25°C))	1.90E-05[a]
Partition Coefficient (log P_{ow})	7.880±0.863[a]
Partition Coefficient (log K_{oc})	5.66[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04).

Known uses: This chemical is marketed as FF-680 by Great Lakes Chemical Corp. for use in HIPS, but is typically used in ABS (Ecology, 2006).

Synonyms: FF 680; FI 680; FireMaster 680; FireMaster FF 680.

Human exposure: No data available**.**

Toxicity: Oral exposure of 1,2-bis(2,4,6-tribromophenoxy)ethane (BTBPE) to rat and dog showed weak acute toxicity (LD > 10g/kg body wt), no obvious effect was seen for rats exposed to BTBPE in the diet for 14 days (Nomeir et al., 1993;RTECS, 2008). Inhalation exposure of BTBPE on rat showed an LC of > 36.68 g/m^3/4 hours, with effects such as behavioral and gastrointestinal changes and dermatitis. Inhalation exposure during three weeks gave a TCLo of 20 g/m^3/4hours/3weeks with effect on lungs, thorax, or respiration (RTECS, 2008). Dermal administration of BTBPE to rabbit showed an LD > 10 g/kg body wt with nutritional and gross metabolic changes (RTECS, 2008).

Eye/skin irritation: 500uL of BTBPE was administered onto the skin of rabbit using the standard draize test and results showed a mild response (RTECS, 2008).

Genotoxicity: The mutagenicity of BTBPE was evaluated in the bacteria Salmonella tester strains TA98, TA100, TA1535, TA1537 and TA1538 (Ames Test) and in the yeast Saccharomyces

cerevisiae tester strain D4, both in the presence and absence of added metabolic activation by Aroclor-induced rat liver S9 fraction. Based on preliminary bacterial toxicity determinations, BTBPE was tested for mutagenicity in the bacterial and yeast cultures at concentrations up to 50 μg/plate. BTBPE did not cause a positive response in any of the bacterial or yeast tester strains, either with or without metabolic activation (Litton Bionetics, 1976).

Endocrine effects: In vitro tests of BFRs for the porfyrinogenic action on chick embryo liver cultures showed no effect from DecaBDE while BTBPE was slightly porfyrinogenic but only after pretreatment with betanaphtoflavone (Koster et al., 1980).

Absorption, distribution and excretion: A study of the metabolism and depuration of ^{14}C BTBPE (Flame retardant: FF-680) in rats was studied. The first group of rats was administered 0.05-5% BTBPE in the diet for 1 day while the second group was given 0.05% for 10 days. The third group of rats was administered a single gavage dose of 200 mg/kg. Results showed that 99% of the total excreted ^{14}C was through the fecal route and 1 % was recovered in the urine. In rats dosed for 10 days only trace levels of radioactivity were found in all tissues except the brain of some animals. The adipose tissue contained the highest levels (excluding the gastrointestinal tract) followed by kidney, skin and thymus and lowest concentrations in brain, testes and spleen. The data indicated that FF-680 where very poorly absorbed through the GI (Nomeir et al., 1993). A metabolization and fate study of BTBPE on rats resulted in >94% of BTBPE exectreted in feces with a minimal retention in tissues. Tissues retaining the highest concentrations were thymus, adipose tissue, adrenals, lung and skin. They concluded that limited absorption and metabolism of BTBPE would occur by ingestion in animals (Hakk and Letcher, 2003;Hakk et al., 2004). Hakk et al. (Hakk et al., 2004) suggested that is possible that an ether cleavage may yield 2,4,6-tribromophenol which have been reported to be an neurotoxicant (Lyubimov et al., 1998).

Bioaccumulation, degradation and fate: A study of Juvenile Rainbow Trout exposed through the diet to BTBPE for 49 days followed by a 154 days depuration showed a linear uptake rate and elimination phase with a depuration half-life of 54.1 days. The determined biomagnifications factor of 2.3 suggested that this chemical have a high potential for biomagnification in the aquatic food web. No metabolites were detected. Biochemical results indicate that BTBPE is not a potent thyroid axis disruptor (Tomy et al., 2007). Biomagnification between trophic levels of the Lake Winnipeg (Canada) food web resulted in a BMF of 0.1-2.5 for BTBPE (Law et al., 2006;Law et al., 2007).

Environmental levels: A study of trophic levels of Lake Winnipeg (Canada) food web found BTBPE with the highest concentration observed in mussels (mean concentration of 1.29 ng/g lipid wt). BTBPE was also detected in Walleye, whitefish and zooplankton. In water the median concentration was 1.96 pg/l (dissolved phase) while the concentration in sediments was below the method detection limit (Law et al., 2006;Law et al., 2007). BTBPE have been found in dust collected from 19

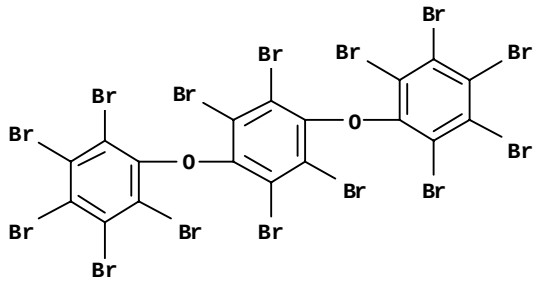
homes in Boston (U.S.) and ranging from 1.6-789 ng/g (Stapleton et al., 2008). BTBPE was also found in herring gull eggs around the Great Lakes in 2004, suggesting that new types of BFRs are present in the aquatic food web of the Great Lakes (Verreault et al., 2007; Gauthier et al. 2008). Lake Ontario sediment cores was investigated and BTBPE was found in the surficial sediment, with average concentration of 6.7 ng/g dry wt (Qiu et al., 2007). BTBPE was also detected in tree bark from the same region in the Northeastern U.S. ranging from ND to 0.62 ng/g bark (Qiu and Hites, 2008). BTBPE have also been reported in the particulate phase in air near the Great Lakes with median concentrations from 0.5 to 1.2 pg/m^3 (Venier and Hites, 2008). BTBPE was detected in air around the Great Lakes in 2002-2003, the authors concluded that these findings correlates with sources of known manufacturing of flame retardants in southern Arkansas. In these regions higher levels of DecaBDE, HBCDD and BTBPE have been observed in air (Hoh and Hites, 2005).
As BTBPE is starting to replace the PentaBDE mixture (Potrzebowksi and Chance, 2004), the importance of monitoring environmental levels is quite significant. The ban of marketing the Penta- and Octa-BDE mixtures (European Union, 2003) may increase the use of BTBPE as well as DBDPE. This may increase the levels found of these compounds in the domestic environment and biota.

Emissions and monitoring data in the Nordic countries: BFRs were determined in air, sedimentary dust and plasma from five households in Sweden. BTBPE was not detected in plasma or air but in sedimentary dust. This is similar to DBDPE, and at the same concentrations as several of the most abundant BFRs (Karlsson et al., 2007).
Among air samples from a plant recycling electronics goods, a factory assembling printed circuit boards, a computer repair facility, and offices equipped with computers, and outdoor air, the highest concentration was found in the electronics recycling plant (mean concentration of 20-150 ng/m^3) while other working environments, such as the printed circuit board factory and offices only had trace levels with an mean concentration of 0.041 and 0.0058 ng/m^3. Outdoor air was below LOQ (Sjodin et al., 2001).
To evaluate exposure to BFR in an electronic recycling facility, personal air monitoring was done for 2 years. A total of 22 PBDEs and 2 other Br-containing organic compounds were analyzed and evaluated in 17 personal air samples (Pettersson-Julander et al., 2004). One of the compounds was identified as BTBPE based on full scan spectra and previous identifications (Sjodin et al., 2001), the other compound was tentatively identified as DBDPE. BTBPE was the second most abundant compound of the BFRs of all samples and was semi-quantitatively determined to <0.6-39 ng/m^3 (Pettersson-Julander et al., 2004).

BTBPE was found in small amounts in northern fulmar eggs from the Faroe Islands (North Atlantic) with a mean concentration of 0.11 ng/g lipid wt. This concentration is 150 times lower than the sumBDEs (Karlsson et al., 2006). BTBPE have also been found in eggs and plasma from glaucous gulls in the Norwegian arctic. Only low concentrations of BTBPE (max 0.96 ng/g lipid wt) were found in egg yolk and in only one plasma sample. Results suggested that BTBPE and other non-BDE BFRs may

undergo long-range atmospheric transport to arctic regions, bioaccumulate (at low concentrations) and are maternally transferred to eggs (Verreault et al., 2007).

4.1.3.3 1,4-Bis(pentabromophenoxy)tetrabromobenzene



Characteristics of the compound:

CAS No.:	58965-66-5
CA Index name:	Benzene, 1,2,4,5-tetrabromo-3,6-bis(2,3,4,5,6-pentabromophenoxy)-
Molecular Formula:	C18 Br14 O2
Molecular Weight (g/mol)	1366.85[a]
Melting Point/range (°C)	Not available
Boiling Point/range (°C)	704.6±60.0[a]
Vapour Pressure (Pa (25°C))	9.2E-17 [a]
Water Solubility (g/l (25°C))	6.00E-13[a]
Partition Coefficient (log P_{ow})	16.481±0.989[a]
Partition Coefficient (log K_{oc})	7.00[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04).

Known uses: Used in engineering thermoplastics.

Synonyms: Benzene, 1,2,4,5-tetrabromo-3,6 bis(pentabromophenoxy) - (9CI); BT 120; BT 120 (fireproofing agent); Pentabromo-1,4-diphenoxybenzene; Saytex 120.

Human exposure: No data available**.**

Toxicity: No data available**.**

Eye/skin irritation: No data available.

Genotoxicity: No data available.

Endocrine effects: No data available.

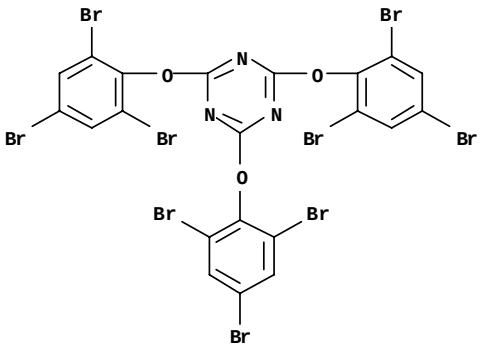
Absorption, distribution and excretion: No data available.

Bioaccumulation, degradation and fate: No data available.

Environmental levels: No data available.

Emissions and monitoring data in the Nordic countries: No data available

4.1.3.4 2,4,6-Tris(2,4,6-tribromophenoxy)-1,3,5-triazine



Characteristics of the compound:

CAS No.:	25713-60-4
CA Index name:	1,3,5-Triazine, 2,4,6-tris(2,4,6-tribromophenoxy)-
Molecular Formula:	C21 H6 Br9 N3 O3
Molecular Weight (g/mol)	1067.43[a]
Melting Point/range (°C)	224[b], 225-235[b], 230[b]
Boiling Point/range (°C)	812.2±75.0[a]
Vapour Pressure (Pa (25°C))	2.7E-23[a]
Water Solubility (g/l (25°C))	8.30E-08[a]
Partition Coefficient (log P_{ow})	12.597±0.949[a]
Partition Coefficient (log K_{oc})	7.00[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04).
b) Data from SciFinder originating from experimentally determined properties.

Known uses: No data available.

Synonyms: s-Triazine, 2,4,6-tris(2,4,6-tribromophenoxy)- (8CI);; FR 245; FR 245 (flame retardant); GX 6145; Pyro-guard SR 245; SR 245; Tris(2,4,6-tribromophenoxy)-s-triazine.

Human exposure: No data available**.**

Toxicity: Practically not toxic to fish up to its limit of water solubility, and not toxic to daphnia up to its limit of water solubility (Pakalin et al., 2007).

Eye/skin irritation: No data available.

Genotoxicity: No data available.

Endocrine effects: No data available.

Absorption, distribution and excretion: No data available.

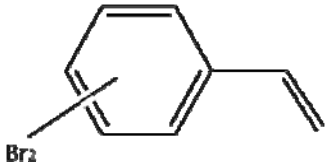
Bioaccumulation, degradation and fate: The substance is considered not inherently biodegradable. The substance was considered to be not bioaccumulative in the food chain: BCFs were determined to be < 0.8-9 and < 8-18 for two concentration ranges (8 weeks study in carps) (Pakalin et al., 2007).

Environmental levels: No data available

Emissions and monitoring data in the Nordic countries: No data available

4.1.4 Polymers/monomers

4.1.4.1 Benzene, ethenyl-, ar-bromo derivatives (Mono-, di- and tri-bromostyrene)



Characteristics of the compound:

CAS No.:	125904-11-2 Dibromostyrene (31780-26-4)	
CA Index name:	Benzene, ethenyl-, ar-bromo derivatives	
Molecular Formula:	Unspecified	
Molecular Weight (g/mol)	Unspecified	
Melting Point/range (°C)	-37[a]	
Boiling Point/range (°C)	95[a]	
Vapour Pressure (Pa (25°C))	9.999 (30°C)[a], 9.999 (25° C)[a]	
Water Solubility (g/l (25°C))	6.91E-03 (20° C)[a]	
Partition Coefficient (log P_{ow})	Monobromostyrene	3.94 (exp)
	Dibromostyrene	4.43 (exp)
	Tribromostyene	4.53 (exp)[a]
Partition Coefficient (log K_{oc})	Monobromostyrene	3.27 (exp)
	Dibromostyrene	3.79 (exp)
	Tribromostyene	4.26 (exp)[a]

a) Experimentally determined data from an IUCLID report of Benzene, ethenyl-, ar-bromo derivs. (US EPA, 2003)

Known uses: Styrenic polymers and engineering plastics.

Synonyms: DBS; Dibromostyrene; CN-19; Step III; Benzene, ethenyl, aryl brominated derivatives; Brominated styrene (US EPA, 2003).

Human exposure: No data available**.**

Toxicity (Dibromostyrene): Dibromostyrene **(**DBS) was administered to 10 male/female Sprague-Dawley rats by a single oral gavage dose. The LD_{50} was determined to 0.050 g/kg corn oil or > 200mg/kg body wt. There was no mortality in the study. This chemical is not considered to be "acutely toxic" (US EPA, 2003). 30 male/female Sprague-Dawley rats was administered three oral single gavage dose levels in corn oil and the animals was observed for toxicity and mortality during 14 days. The LD_{50} was determined to 6327 g/kg body wt. Toxic effects included ataxia, lethargy, prostration, lacrimation, and urine stains. Pathological findings included stomach distended with food, forestomach with shaggy white or chalky white material, hindstomach reddened or pale with or without focal hemorrhage,

and intestines reddened (US EPA, 2003).

Inhalation studies with doses of 2 mg/l for 1h where performed on 10 male Sprague-Dawley rats. The rats where observed for 2 days, and results showed an LC of >3.1 mg/l. No mortalities where reported in the study. DBS was not considered acutely toxic by the inhalation route (US EPA, 2003).

Dermal toxicity was evaluated on 10 male/female New Zealand albino rabbits. DBS was administered at a dose of 2 g/kg body wt for 24h. No mortality was observed during this time frame resulting in a LD_{50} of > 2g/kg body wt. (US EPA, 2003).

Acute toxicity in male/female Crl:CD® BR rats was studied. DBS was continuously administered for 28 days during an oral dose range finding study in the concentration range of 200-1600 mg/kg body wt/day. Some evidence of systemic toxicity where observed at 1600 mg/kg body wt, clinical signs of toxicity where observed in the 300 and 800 mg/kg body wt dose group while no effects where observed in the 200mg/kg group. Nine of ten animals dosed at 200mg/kg for 21 days and later increased to 2400mg/kg died within 3 days of the initial higher dose. No valid NOAEL was achieved in this study.(US EPA, 2003).
DBS was administered during 28 days by an oral gavage dose of 1-100mg/kg/day in a range finding study on Sprague-Dawley rats. No mortality was observed and no effects were observed that could be contributed to treatments observed in the study. They determined a NOAEL of 100mg/kg body wt (US EPA, 2003). A 90 day subcronic toxicity study was performed on Crl:CD® BR male and female rats at concentrations from 130-1600 mg/kg body wt/day. The recovery period was 4 weeks. The study shows systemic and clinical signs of toxicity. They reported a NOAEL of 130 mg/kg body wt and a LOAEL of 300 mg/kg body wt (US EPA, 2003).

The toxicity to reproduction after exposure to DBS was studied in male/female Sprague-Dawley rats. The exposure period was 70 days with two generations and with an oral (gavage) administration of 100-1600 mg/kg/day. Results indicated potential adverse effects of DBS on the reproductive capabilities of the F0 and F1 generations and neonatal viability and growth. Potential adverse effect on fertility was observed in F1 males at 1600mg/kg. No other adverse effects on reproductive parameters were observed in the F0 and F1 generations at any dose. Results from the study showed an NOAEL (Parental) of 100 mg/kg body wt, NOAEL (F0 offspring) of < 100 mg/kg body wt and NOAEL (F1 offspring) of 400 mg/kg body wt (US EPA, 2003).

A developmental toxicity/teratogenicity study was made on female New Zealand white rabbits. DBS was administered by oral gavage doses of 50-700mg/kg/day during exposure gestation day 7-19, duration of test gestation day 29. Four deaths occurred at 700 mg/kg and three deaths at 500mg/kg, significant maternal mean body weight losses and reduced food consumption at 700 and 500mg/kg. Results showed no developmental toxicity of DBS, the maternal NOAEL was determined to 250mg/kg body wt and the teratogen NOAEL to 500 mg/kg body wt (US EPA, 2003).

Another study performed with a concentration range of 25-350 mg/kg/day resulten in maternal toxicity such as mortality, clinical signs, weight loss and decreased food consumption was evident at 350 mg/kg/day. The maternal NOAEL was determined to be 150 mg/kg body wt and the teratogen NOAEL to be 250 mg/kg body wt (US EPA, 2003).
The potential maternal and developmental toxicity in rats was studied. DBS was administered through oral gavage doses on female Crl:CD(R)BR rats at 100-1600mg/kg/day. No mortalities occurred but some signs of maternal toxicity were observed for the doses of 800 and 1600mg/kg. Foetal developmental effects were on weight and some external defects. Maternal NOAEL was determined to be 400 mg/kg body wt and teratogen NOAEL to be 800 mg/kg body wt (US EPA, 2003).
In another study at the same concentration range and with the same type of rat, maternal mortality (5 out of 25) was shown at 1600mg/kg. Clinical signs appeared at doses of 400mg/kg and higher, while food consumption and weight gain where inhibited at doses >100mg/kg. Maternal clinical toxicity observed in this study. Adverse effects on the developing fetuses such as reduced body weight and post-implantation loss appeared at 1600mg/kg, effect on the morphological development was observed from 400-1600mg/kg and external malformations at 1600mg/kg. Maternal toxicity was noted at all doses. Maternal NOAEL was <100 mg/kg body wt and teratogen NOAEL of 100 mg/kg body wt (US EPA, 2003).

Eye/skin irritation: 6 rabbits were exposed using the standard draize test during 24h for 0.5ml of DBS. A primary dermal irritation of 6.6 classified DBS as severely irritating. In another test, exposure for 0.5 mL for 4hours resulted in an index of 4.1, moderately irritating. BDS was not considered to be corrosive (US EPA, 2003).

Exposure of 9 rabbits to 0.1ml DBS instilled into the cojunctival sac of the right eye for 0.5min, gave a primary irritation index of 11.00, which classify BDS as mildly irritating. Exposure of 6 rabbits to 0.1mL DBS instilled into the cojunctival sac of the right eye but not rinsed resulted in a primary irritation index of 7.3 at 1hour, which classify BDS as slightly irritating (US EPA, 2003).

A 5 week study on the DBS dermal sensitization potential was studied on Guinea pigs. Only a slight reaction was observed for 5 out of 8 animals resulting in a classification of DBS as not being an sensiti-zing agent on guinea pig (US EPA, 2003).

Genotoxicity: The Ames test was preformed using Salmonella strains with an incorporation of 0.001-0.50 µl/plate, with and without metabolic activation. Results showed no genetic activity in any of the assays tested. DBS was considered not mutagenic (US EPA, 2003). A mammalian cell gene mutation test of DBS was performed on CHO/HGORT cells at a concentration of 5-25 nl/ml without metabolic activation and 25-70 nl/ml with metabolic activation. DBS was found to be negative in the CHO/HGPRT mutation assay (US EPA, 2003). The effect of DBS on the unscheduled DNA synthesis on rat primary hepatocytes was studied. DBS was tested in the concentration range of

0.001-0.03 µl/ml, with and without metabolic activation. DBS did not cause a significant increase in net nuclear grain counts at any dose level (US EPA, 2003).

The chromosomal aberration test was performed on Chinese hamster ovary (CHO) cells at concentrations of 0.005-0.04 µl/ml with and without metabolic activation (Aroclor-induced rat liver S-9). A statistical significant increase of chromosome aberration was observed at 0.01 and 0.005 µl/ml in the non activated test and 0.03µl/ml in the activated test (US EPA, 2003). DBS was considered a suspected positive in the CHO chromosome aberration test (US EPA, 2003). The chromosomal aberration test was performed on Chinese hamster ovary (CHO) cells in two rounds at a concentration of 1-15 µg/ml and 2.5-35 µg/ml, and the metabolically activated concentration ranges were 5-75 µg/ml and 9-90 µg/ml. The highest concentration, 90 µg/ml (metabolically activated), had a statistically significant increase in aberration/cell while all other concentration ranges was found to be negative for chromosome aberration. The investigators concluded that DBS was negative in the CHO chromosome aberration test (US EPA, 2003).

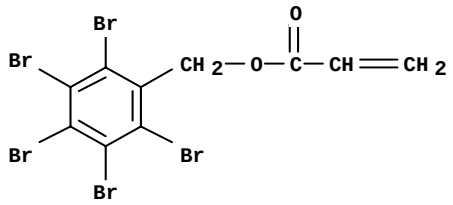
Absorption, distribution and excretion: No data available.

Bioaccumulation, degradation and fate: Experimental testing of mono, di and tri-bromostyrene showed a log K_{oc} value 3.27-4.26. Based on these data the test substances are expected to absorb to soil and not to partition to other compartments (US EPA, 2003). Hydrolysis of DBS was studied experimentally in an aqueous buffer medium (pH 4, 7, 9) at 1 mg/l during 5 days at temperatures of 15 and 25°C, DBS was hydrolytically stable at 15°C (pH 4 and 7) but not at pH 9, while at 25°C (all pH ranges) it was hydrolysed. This results in estimated half-lives of mono, di and tri-bromostyrene of 39-43, 50-59 and 37-49 days, respecively(US EPA, 2003).

Environmental levels: No data available.

Emissions and monitoring data in the Nordic countries: No data available.

4.1.4.2 Pentabromobenzyl acrylate



Characteristics of the compound

CAS No.:	59447-55-1
CA Index name:	2-Propenoic acid, (2,3,4,5,6-pentabromo phenyl)methyl ester
Molecular Formula:	C10 H5 Br5 O2
Molecular Weight (g/mol)	556.67[a]
Melting Point/range (°C)	Not available
Boiling Point/range (°C)	477.7±40.0[a]
Vapour Pressure (Pa (25°C))	3.64E-07[a]
Water Solubility (g/l (25°C))	1.40E-03[a]
Partition Coefficient (log P_{ow})	5.463±0.637[a]
Partition Coefficient (log K_{oc})	4.35[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04).

Known uses: Polybutyleneterephatlate (PBT), Polyethylene terephthalate (PET) and ABS plastics.

Synonyms: 2-Propenoic acid, (pentabromophenyl)methyl ester (9CI); 2,3,4,5,6-(pentabromophenyl)methyl acrylate; Actimer FR 1025M; FR 1025M.

Human exposure: No data available**.**

Toxicity: No data available**.**

Eye/skin irritation: No data available.

Genotoxicity: No data available.

Endocrine effects: No data available.

Absorption, distribution and excretion: No data available.

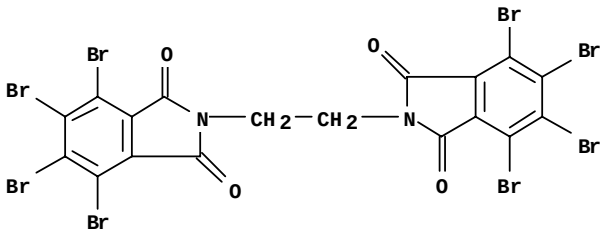
Bioaccumulation, degradation and fate: No data available.

Environmental levels: No data available.

Emissions and monitoring data in the Nordic countries: No data available

4.1.5 Other

4.1.5.1 Ethylene bis(tetrabromophthalimide)



Characteristics of the compound:

CAS No.:	32588-76-4
CA Index name:	1H-Isoindole-1,3(2H)-dione, 2,2'-(1,2-ethanediyl) bis[4,5,6,7-tetrabromo-
Molecular Formula:	C18 H4 Br8 N2 O4
Molecular Weight (g/mol)	951.47[a]
Melting Point/range (°C)	Not available
Boiling Point/range (°C)	827.9±65.0[a]
Vapour Pressure (Pa (25°C))	1.97E-25[a]
Water Solubility (g/l (25°C))	2.60E-05[a], 3.0E-12[b]
Partition Coefficient (log P_{ow})	7.561±0.855[a], 9.80[b]
Partition Coefficient (log K_{oc})	5.49[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Estimated in EPIWin (Hardy et al., 2002)

Known uses: Ethylene bis(tetrabromophthalimide) (EBTPI) is an additive flame retardant. It finds use in polyolefins, high-impact polystyrene (HIPS), thermoplastic polyesters (PBT, PET, etc.), polycarbonate and elastomers whose applications include electrical and electronics components, wire and cable insulation, switches, and connectors (TOXNET, 2008).

Synonyms: 1,2-Bis(tetrabromophthalimido)ethane; Phthalimide, N,N'-ethylenebis[tetrabromo- (8CI); N,N'-Ethylenebis(tetrabromophthalimide); BT 93; BT 93W; BT 93WFG; Citex BT 93; N,N'-Ethylenebis(tetrabromophthalimide); Saytex BT 93; Saytex BT 93W

Human Exposure: Occupational exposure to ethylene bis tetrabromophthalimide (EBTPI) may occur through inhalation and dermal contact with this compound at workplaces where EBTPI is produced or used. Occupational exposure would be expected to be minimal, since ethylene bis(tetrabromophthalimide) is manufactured in a closed system (TOXNET, 2008).

Toxicity: Oral administration of EBTPI to rat gave an LD50 of >7500 mg/kg, effects was not reported (RTECS, 2008).

EBTPI has a NOEL in rat and rabbit of 1000 mg/kg body wt during an 90 day study (US EPA, 2004b).

An inhalation study on rat gave a LC >203 g/kg/m^3/1 hour, with effects on sense organs (olfaction) and the respiratory system (dyspnea and pulmonary emboli).
EBTPI was dermally administered to rabbit, with a LD50 >2g/kg (effects not reported) (RTECS, 2008).

Developmental or reproductive toxicity where studied using Saytex BT 93 (EBTPI) and administered to two groups of 20 mated female New Zealand White rabbits each by gavage at a dose of 0 or 1,000 mg/kg/day on gestation days 7-19. The females were sacrificed on gestation day 29 and subjected to a cesarean section. No maternal mortality, abortions or clinical signs of toxicity were observed during the study. Maternal body weights, weight gain, food consumption, necropsy observations and cesarean section data were generally comparable among the groups. No treatment-related malformations or developmental variations in the fetuses were observed. The maternal and fetal NOEL was 1,000 mg/kg/day (TOXNET, 2008).

Eye/skin irritation: Standard draize test performed with rabbit, administration into the eye with a dose of 100mg/24 hours, resulted in a mild reaction to EBTPI (RTECS, 2008).

Genotoxicity: Mutagenicity was tested in the Ames *Salmonella typhimurium* strains with and without metabolic activation. No mutagenic activity was found for any of the tested chemicals (Zeiger et al., 1985).

Endocrine effects: EBTPI was shown to be slightly porfyrinogenic at 10 ug/ml in chick embryo but only after pretreatment with beta-naphtoflavone (Koster et al., 1980).

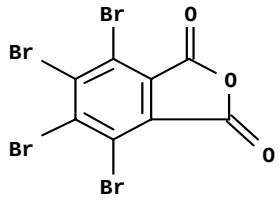
Absorption, Distribution & Excretion: A mammalian pharmacokinetic study indicates that 85% of the total dose administered over a 14 day period was recovered in the feces and urine with a short half-life of < 17-20 days. This suggests that EBTPI is not able to bioaccumulate (TOXNET, 2008).

Bioaccumulation, degradation and fate: EBTPI was not readily biodegradable by activated sewage sludge over a 2-day period when tested under Japanese MITI/OECD Ready Biodegradability 301C Modified MIT1 guidelines (US EPA, 2004b). The BCF was studied in the Japanese Carp according to OECD guidelines (305C). No bioconcentration was observed for EBTPI during the 6 week study (BCF = <0.3 to <33) (Hardy, 2004).

Environmental levels: No environmental levels have to our knowledge been reported for EBTPI.

Emissions and monitoring data in the Nordic countries: No data available.

4.1.5.2 Tetrabromophtalic anhydride



Characteristics of the compound:

CAS No.:	632-79-1
CA Index name:	1,3-Isobenzofurandione, 4,5,6,7-tetrabromo-
Molecular Formula:	C8 Br4 O3
Molecular Weight (g/mol)	463.70[a]
Melting Point/range (°C)	274-275[b], 278-280[b]; 279.5-280.5[b]
Boiling Point/range (°C)	540.5±50.0[a]
Vapour Pressure (Pa (25°C))	1.27E-9[a]
Water Solubility (g/l (25°C))	2.4E-02[a]
Partition Coefficient (log P_{ow})	3.779±0.698[a]
Partition Coefficient (log K_{oc})	3.43[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Data from SciFinder originating from experimentally determined properties

Known uses: Unsaturated polyesters and rigid polyurethane foams, paper, textiles, epoxides and wool.

Synonyms: Phthalic anhydride, tetrabromo- (6CI,7CI,8CI); 3,4,5,6-Tetrabromophthalic anhydride; Bromphthal; FG 4000; FireMaster PHT 4; NSC 4874; PHT 4; Saytex RB 49; Tetrabromophthalic acid anhydride.

Human exposure: 50 males and females subjected to induction patches of tetrabromophtalic anhydride on the upper back and upper arm for 9 weeks exhibited no oedema, erythema or skin senzitation (Tice and Masten, 1999).

Toxicity: Oral administration to rat resulted in a LD_{50} >10g/kg, no details on effects were reported (RTECS, 2008).

An inhalation study on rat of tetrabromophtalic anhydride resulted in a LC of >10.92 g/m^3/4 hours and toxic effects resulting in changes in motor activity. Another study showed an LCLo of 2 g/m^3/4 hour/3 weeks (intermittent), with pathologial effects on lung weight, changes in structure or function of salivary glands and changes in liver weight. Another study resulted in a lowest observed toxicity of 50ug/m^3/5 days (intermittent), resulting in a increase in humoral immune response (RTECS, 2008).

Dermal administration of tetrabromophthalic anhydride on rabbit resulted in a determined LD_{50} of >10 g/kg with behavioural effects such as somnolence and a general depressed activity. Similarly, dermal administration on guinea pig resulted in a LD_{50} of >1 g/kg (no details on effect). Another study on rabbit resulted in a lowest observed toxicity of 100 g/kg/4 weeks (intermittent), resulting in behavioural effects such as ataxia, weight loss or decreased weight gain and death (RTECS, 2008).

Eye/skin irritation: In a standard draize test on rabbit, 100 mg tetrabromophtalic anhydride was administratered into the eye resulting in a mild reaction (RTECS, 2008). Another test using the standard draized test on rabbit found the chemical not to be an eye irritant (Tice and Masten, 1999).

Genotoxicity: Tetrabromophtalic anhydride was found to be non-mutagenic in the Ames Salmonella typhimurium mutagenicity test with and without metabolic activation (MacGregor and Friedman, 1977;Zeiger et al., 1985)

Endocrine effects: Examination of receptor binding and activation by BFRs through the Ah receptor reporter gene assay demonstrated the ability of Firemaster PHT4 (primary constituent Tetrabromophthalic anhydride) to bind to the Ah receptor to levels comparable to TCDD and results showed that Firemaster PHT4 was able to stimulate AhR dependent gene expression at moderate to high concentrations. The level of induction shown in this test is similar to many other BFRs (Brown et al., 2004). Screening of some anti-androgenic endocrine disruptors revealed tetrabromophtalic anhydride to be inactive as an anti-androgen in the Chinese hamster ovarian cell line (Roy et al., 2004).

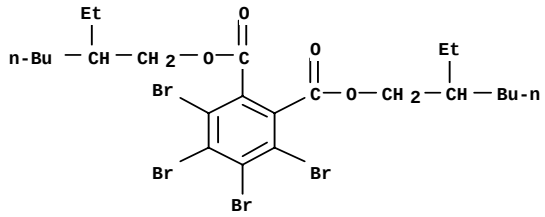
Absorption, distribution and excretion: 75 % of the tetrabromophtalic anhydride was excreted in the feces, while the amount absorbed by the gastrointestinal tract was rapidly excteted in the urine. The retention half-life was < 7 hours. Tetrabromophtalic anhydride was not expected to persist or bioaccumulate (Tice and Masten, 1999).

Bioaccumulation, degradation and fate: tetrabromophtalic anhydride was proposed to be one of 120 high production chemicals which are structurally similar to known arctic contaminants and/or have partitioning properties that suggests they are potential arctic contaminants (Brown and Wania, 2008).

Environmental levels: No reported studies in the peer reviewed literature.

Emissions and monitoring data in the Nordic countries: No data available.

4.1.5.3 Bis(2-ethylhexyl)tetrabromophtalate



Characteristics of the compound:

CAS No.:	26040-51-7
CA Index name:	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1,2-bis(2-ethylhexyl) ester
Molecular Formula:	C24 H34 Br4 O4
Molecular Weight (g/mol))	706.14[a]
Melting Point/range (°C)	Not available
Boiling Point/range (°C)	584.8±45.0[a]
Vapour Pressure (Pa (25°C))	1.55E-11[a]
Water Solubility (g/l (25°C))	1.60E-06[a]
Partition Coefficient (log P_{ow})	10.084±0.938[a]
Partition Coefficient (log K_{oc})	6.86[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04)

Known uses: bis(2-ethylhexyl)tetrabromophtalate (TBPH) has reportedly been used as a plasticizer in polyvinylchloride (PVC) and neoprene (Andersson et al., 2006) and is currently marketed for use as a flame retardant plasticizer for PVC applications such as wire and cable insulation, coated fabrics, film and sheeting (Great Lakes, 2004).

Synonyms: 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, bis(2-ethylhexyl) ester (9CI); Phthalic acid, tetrabromo-, bis(2-ethylhexyl) ester (8CI); DP 45; Di(2-ethylhexyl) tetrabromophthalate; Pyronil 45; Uniplex FRP 45, Firemaster 550.

Human exposure: No data available.

Toxicity: No data available**.**

Eye/skin irritation: No data available.

Genotoxicity: No data available.

Endocrine effects: No data available.

Absorption, distribution and excretion: No data available.

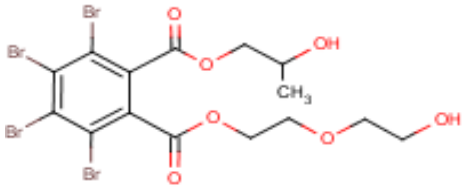
Bioaccumulation, degradation and fate: No data available.

Environmental levels: Dust collected from 19 homes in Boston, Massachusetts, showed TBPH and the decarboxylated form of TBPH which was

identified to be 2-ethylhexyl-2,3,4,5-tetrabromobenzoate (TBB) and the dominant brominated compound in Firemaster 550. TBPH was detected in house hold dust at ranges 1.5-10600 ng/g dust wt at levels comparable to HBCDD (Stapleton et al., 2008).
TBPH and TBB was further detected in biosolids from two San Francisco bay area waste water treatment plants (WWTP) ranging from 40 to 1412 ng/g dry wt and 57 to 515 ng/g dry wt, respectively (Klosterhaus et al., 2008). Firemaster 550 is a replacement product for PentaBDE (Venier and Hites, 2008;Chemtura, 2008) and was introduced to the market in 2003 (Stapleton et al., 2008).

Emissions and monitoring data in the Nordic countries: No data available.

4.1.5.4 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester



Characteristics of the compound:

CAS No.:	20566-35-2 (earlier 77098-07-8)
CA Index name:	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1-[2-(2-hydroxyethoxy)ethyl] 2-(2-hydroxypropyl) ester
Molecular Formula:	C15 H16 O7 Br4
Molecular Weight (g/mol)	627.90[a]
Melting Point/range (°C)	Not available
Boiling Point/range (°C)	598.5±50.0[a]
Vapour Pressure (Pa (25°C))	9.81E-13[a], 3.12E-12[b]
Water Solubility (g/l (25°C))	0.88[a], 5.0E-05[b]
Partition Coefficient (log P_{ow})	1.152±0.996[a], 3.82[b]
Partition Coefficient (log K_{oc})	2.0[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Estimated in EPIWin v3.04

Known uses: No data available.

Synonyms: SaytexB RB-79; Great Lakes PHT4-Diol; TBPA Diol.

Human exposure: No data available

Toxicity: Five male and 5 female Sprague-Dawley rats were orally administered a single dose of TBPA diol at a concentration of 10g/kg body wt and observed during 14 days. No deaths occurred in this test, and LC_{50} was >10g/kg body wt (US EPA, 2004a).

Two female New Zealand albino rabbits were dermally administrered 20 g/kg of TBPA diol for a 24 hour exposure period and the animals was observed for 14 days. Body weight was monitored, no effect was observed and no animals died during this time period. The dermal LD_{50} was > 20 g/kg (US EPA, 2004a).

Five female Charles River CD rats were administered 8 mg/m^3 TBPA diol through the inhalation route during an one hour exposure period. Observations were made for 14 days post dosing and body weight was recorded. No deaths occurred during this period. Animals

were necropsied at the end of day 14 and no signs of toxicity were observed. LC50 was > 0.008 mg/kg/1 hour (US EPA, 2004a).

Eye/skin irritation: TBPA diol was instilled into the right eyes of six rabbits, and observed during 72 hours. No positive ocular scores were recorded. TBPA were not irritating to the eye. 0.1 ml of TBPA diol were administered into the conjunctival sac of the right eyes of three male and three female New Zealand albino rabbits. Redness and chemosis of the conjunctiva were observed for 72h. Discharge was noted in one of the rabbits at 24h. They concluded that TBPA diol was not a primary irritant under the conditions of this test(US EPA, 2004a). Skin irritation test was made according to the Draize test on three female and three male New Zealand albino rabbits. 0.5 ml of TBPA diol was applied, and the skin was observed for 72 hours. No irritation was observed on the intact skin while erythema and edema was observed on the abraded skin. The primary irritation index (Draize method) was 0.7. They concluded that TBPA diol was not a primary skin irritant under the conditions of this test(US EPA, 2004a).

Bluegill sunfish (Lepomis macrochirus) was exposed for 96 hours to concentrations of 0-100 mg/l showing an LC_{50} of 12 mg/l/96 hours (US EPA, 2004a).

Genotoxicity: TBPA diol was tested in *Salmonella tyhpimurium* strains with and without metabolic activation. Dose levels were 0-5000 μg/plate. The dose related increase of TBPA diol did not cause an increase in mutant colonies in any strain, with or without metabolic activation. They concluded that TBPA diol was not genetically active.

TBPA diol was examined for mutagenic activity on *Salmonella* and *Saccharomyces* organisms with and without metabolic activation. TBPA diol was not found to be mutagenic (US EPA, 2004a).

Endocrine effects: No data available.

Absorption, distribution and excretion: No data available.

Bioaccumulation, degradation and fate: TBPA diol is not expected to bioconcentrate and its estimated chronic toxicity value in fish is below that of its estimated water solubility (calculated in EPIwin v 3.04, PBT profiler) (US EPA, 2004a). They conclude that TBPA diol is not expected to concentrate in higher organisms to a level that might be toxic.

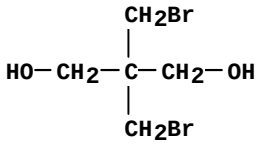
Environmental levels: No data available.

Emissions and monitoring data in the Nordic countries: No data available.

4.2 Alifatics

4.2.1 Alcohols

4.2.1.1 Dibromoneopentyl glycol



Characteristics of the compound:

CAS No.:	3296-90-0
CA Index name:	1,3-Propanediol, 2,2-bis(bromomethyl)-
Molecular Formula:	C5 H10 Br2 O2
Molecular Weight (g/mol)	261.94[a]
Melting Point/range (°C)	112-114[b], 111-113[b], 109[c]
Boiling Point/range (°C)	370.9±42.0[a] 134 (at 133.332 Pa)[d]
Vapour Pressure (Pa (25°C))	5.16E-07[a] 133 (129.7°C) (FR-1138)[d] 5333 (213.6°C) (FR-1138)[d] 1333 (178°C) (FR-522)[d] 3333 (200°C) (FR-522)[d]
Water Solubility (g/l (25°C))	34[a], 38[c]
Partition Coefficient (log P_{ow})	0.385±0.543[a], 1.1[d], 1.06[d], 2.29[c]
Partition Coefficient (log K_{oc})	1.59[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Data from SciFinder originating from experimentally determined properties
c) Data from the HSDB data sheet available from TOXNET (TOXNET, 2008)
d) Data from a report by the Danish EPA (Simonsen et al., 2000)

Known uses: Reactive flame retardant for epoxy, polyester and urethane foams. Chemical intermediate for pentaerythritol ethers and for derivatives used as flame retardants (TOXNET, 2008).

Synonyms: 1,3-Dibromo-2,2-dihydroxymethylpropane; 2,2-Bis(bromomethyl)-1,3-propanediol; 1,3-Dibromo-2,2-dimethylolpropane; 2,2-Dibromomethyl-1,3-propanediol; Dibromoneopentyl glycol; FR 1138; FR 522; NSC 9001; Pentaerythritol dibromide; Pentaerythritol dibromohydrin; Pentaerythritol dibromide.

Human Exposure: Occupational exposure to Dibromoneopentyl glycol

(DBNPG) may occur through inhalation and dermal contact with this compound at workplaces where DBNPG is produced or used (TOXNET, 2008).

Toxicity: Oral administration of DBNPG to rat and mouse gave LD50 of 1880 mg/kg and 1200 mg/kg, respectively. No information on toxic symptoms or histological changes was reported. Multiple dose toxicity during 13 weeks through oral administration to rat gave a lowest observed toxic dose of 109 g/kg/13 weeks. The toxic effects reported were on the kidney with changes in tubules, including acute renal failure, acute tubular necrosis, and weight loss or decreased weight gain. Another study showed a lowest observed toxic dose for an oral administration to rat of 9g/kg/30 days giving changes in liver weight. One 2 year study showed a lowest observed toxic dose of 73g/kg/2 years with effects on sense organs (eyes) (RTECS, 2008). Toxicity studies for oral administration of DBNPG on mouse gave a lowest observed toxic dose of 36 g/kg/13 weeks and 3836 mg/kg/14 days with effect on kidneys and weight loss or decreased weight gain (RTECS, 2008).
Groups of Sprague-Dawley rats were maintained on diets supplying nominal doses of 0, 5 or 100 mg DBNPG (FR-1138)/kg body wt/day for up to two years. Toxic effects were observed at the high dose level in liver, lenses of the eyes, and thyroids. Chemical exposure caused neoplasms of the skin, subcutaneous tissue, mammary gland, Zymbal's gland, oral cavity, oesophagus, forestomach, small intestine, large intestine, mesothelium, kidney, urinary bladder, lung, thyroid gland, seminal vesicle, haematopoietic system, and pancreas in the male rat; mammary gland, oral cavity, oesophagus, and thyroid gland in the female rat. The NOAEL was 5 mg/kg body wt/day, and no evidence of FR-1138 related carcinogenicity was observed. DBNPG was administered in the feed to B6C3F1 mice (60/sex/dose level) for 2 years at concentrations of 0, 312, 625, and 1,250 ppm. NOAEL was 312 ppm for males and could not be established for females because of treatment related neoplastic effects observed from the lowest dosage level in the Harderian gland. Chemical exposure caused toxic effects on lung, kidney, and the Harderian gland in male mice; and effect on subcutaneous tissue, lung, and Harderian gland in the female mouse. The recovery group of male rats presented with the same spectrum of treatment-related neoplasms as in the core study. In this recovery group, DBNPG (at 20,000 ppm) caused irreversible effects at numerous sites after 13 weeks of exposure that was not detectable by histological examination, but without further exposure eventually resulted in the development of neoplasms at multiple sites (Simonsen et al., 2000).
Adminstration through inhalation to rats of the flame retardant FR-1138 (Purity: 81.1%) for vapours with a concentration of 2.49 mg/l for a period of 7 hours resulted in slightly laboured breathing and slight nasal irritation but no mortality(Simonsen et al., 2000).

Eye/skin irritation: Administration of DBNPG on intact skin and eye of 6 rabbits showed no effect on skin, while BDNPG was slightly irritating to the eye (Simonsen et al., 2000).
The skin sen-sitising potential of DBNPG (FR-1138) was evaluated in male guinea pigs by two methods very sparsely reported. No evidence of FR-1138 related skin sensiti-zation was observed (Simonsen et al., 2000).

Genotoxicity: A gene Mutation test was made for DBNPG using an in vitro assay with the Salmonella typhimurium strains (TA-98, TA-1535, TA-1537 and TA-1538) and Saccharomyces cerevisiae. DBNPG was tested with and without metabolic activaton using Aroclor-induced hamster or rat liver (S-9 mix). DBNPG was considered negative in this test while the TA-100 strain was tested positive after metabolic activation. Further, DBNPG was tested negative on the Chinese Hamster ovary cell assay and positive after metabolic activation (TOXNET, 2008).

The chromosome aberrations in Chinese Hamster Ovary cells with and without metabolic acti-vation (+/- S-9 mix) resulted in very slight increase in chromosome aberration at toxic concentrations and metabolic activation. Sister chromatid exchanges with and without metabolic activation was negative without S-9 and positive with metabolic activation (Galloway et al., 1987).

DBNPG was administered to rats for 1-2 years and was shown to be carcinogenic at levels of 72.8 to 108 g/kg/year, giving tumors on skin and appendages, lungs, thorax or respiration, thyroid tumors and leuk-emia. A 2 year study of oral administration of DBNPG to mouse at levels of 51-54 g/kg/year showed a possible carcinogenic effect of DBNPG to lungs, thorax or respiration (RTECS, 2008). Oral administration of DBNPG for 2 years resulted in carcinogenicity for rat and mouse. In male Medaka DBNPG was found to be carcinigenic while the respons was negative in females. Female and male Guppies gave also a positiv respons for DBNPG (TOXNET, 2008).

Endocrine effects: No data available.

Reproductive effects: Oral administration of 62 g/kg body wt and 124 g/kg body wt of DBNPG to male mouse during 15 weeks pre-mating showed reproductive effects, while female mouse administered 62 g/kg, 15 weeks pre-mating, showed effect on fertility and effects on newborn (RTECS, 2008).

Absorption, distribution and excretion: No data available.

Bioaccumulation, degradation and fate: Aerobic biodegradation on DBNPG, present at 100 mg/l, reached 3 to 33% of its theoretical BOD in 28 days using an activated sludge inoculum at 30 mg/l in the Japanese MITI test (Simonsen et al., 2000).
BCF values of 0.8 to 1.1 and <4.8 were measured for DBNPG at concentrations of 3 mg/l and 0.3 mg/l, respectively, in a 6 week study using carp. According to a classification scheme, these BCF values suggest that the potential for bioconcentration in aquatic organisms is low(Simonsen et al., 2000).

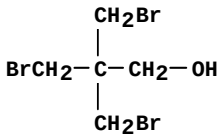
The Hazardous Substanse Data Bank (HSDB) concluded that based on available information and calculated data 2,2-Bis(bromomethyl)-1,3-propanediol's production and use as a reactive flame retardant may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of $1.73x10^{-3}$ Pa at 25 °C indicates DBNPG will exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase DBNPG will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 2 days. Particulate-phase DBNPG will be re-

moved from the atmosphere by wet and dry deposition. If released to soil, DBNPG is expected to have moderate mobility based upon an estimated K_{oc} of 420. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 4.15 x 10^{-4} Pa-m^3/mole. No data were located showing the biodegradation of this compound in the environment; however, only 3 to 33% biodegradation of this compound was reported in 28 days in a screening biodegradation test suggesting that biodegradation of this compound in soil and water may be slow. If released into water, DBNPG may adsorb to suspended solids and sediment based upon the estimated K_{oc}. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. BCF values ranging from 0.8 to 4.8 suggest bioconcentration in aquatic organisms is low. Occupational exposure to DBNPG may occur through inhalation and dermal contact with this compound at workplaces where DBNPG is produced or used (TOXNET, 2008).

Environmental levels: No data available.

Emissions and monitoring data in the Nordic countries: No data available.

4.2.1.2 Tribromoneopentyl alcohol (1-Propanol, 2,2-dimethyl-, tribromo deriv.)



Characteristics of the compound:

CAS No.:	1522-92-5 (or 36483-57-5)
CA Index name:	1-Propanol, 3-bromo-2,2-bis(bromomethyl)-
Molecular Formula:	C5 H9 Br3 O
Molecular Weight (g/mol)	324.84[a]
Melting Point/range (°C)	90-95[b], 66-67[b]
Boiling Point/range (°C)	330.7±42.0[a] 130-135 (at 40 Pa)[b] 170-180 (at 1.6E03 Pa)[b]
Vapour Pressure (Pa (25°C))	1.60E-03[a]
Water Solubility (g/l (25°C))	2.20[a]
Partition Coefficient (log P_{ow})	2.469±0.451[a]
Partition Coefficient (log K_{oc})	2.72[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Data from SciFinder originating from experimentally determined properties

Known uses: TBNPA is used as a reactive intermediate for high molecular weight flame retardants, e.g. polyurethanes and is abundant in bromine chemical industries (OECD, 1994).

Synonyms: 2,2,2-Tris(bromomethyl)-ethanol; 3-Bromo-2,2-bis(bromomethyl)propanol; 2,2-Bis(bromomethyl)-3-bromo-1-propanol; 3-Bromo-2,2-bis(bromomethyl)-1-propanol; 3-Bromo -2,2-bis(bromomethyl)propyl alcohol; FR 1360; FR 513; NSC 20521; Pentaerythritol tribromohydrin; Pentaerythritol tribromide.

Human Exposure: No data available

Toxicity: No data available**.**

Skin/eye irritation: No data available.

Genotoxicity: TBNPA was tested for mutagenicity in the Salmonella/microsome preincubation in five Salmonella typhimurium strains (TA97, TA98, TA100, TA1535, and TA1537) in the presence and absence of Aroclor-induced rat or hamster liver S9. These tests were positive at a dose of 3 µg/plate (Mortelmans et al., 1986).

Endocrine effects: No data available.

Absorption, distribution and excretion: No data available.

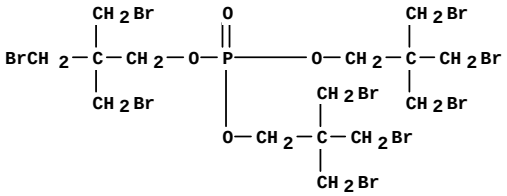
Bioaccumulation, degradation and fate: No data available.

Environmental levels: TNBPA was the most abundant pollutant in the vadose zone and local chalk aquitard of the Northern Negev Desert, Israel. A reaction kinetics study showed that three different decomposition product where produced: 3-bromomethyl-3-hydroxymethyloxetane, 2,6-dioxaspiro[3.3] heptanes and 3,3-bis(bromomethyl)oxetane, of which the chlorinated counterpart is included in the US-EPA list of extremeely hazardous chemicals. They estimated the half-life of TNBPA to be approx 100 years, suggesting that TNBPA is persistent in the aquatic environments (Ezra et al., 2005;Ezra et al., 2006).

Emissions and monitoring data in the Nordic countries: No data available.

4.2.2 Halogenated organophosphorous flame retardant

4.2.2.1 Tris(tribromoneopentyl) phosphate



Characteristics of the compound:

CAS No.:	19186-97-1
CA Index name:	1-Propanol, 3-bromo-2,2-bis(bromomethyl)-, 1,1',1"-phosphate
Molecular Formula:	C15 H24 Br9 O4 P
Molecular Weight	1018.46[a]
Melting Point/range (°C)	175-178[b], 180-182[c]
Boiling Point/range (°C)	719.3±60.0[a]
Vapour Pressure (Pa (25°C))	1.41E-17[a]
Water Solubility (g/l (25°C))	1.80E-05[a]
Partition Coefficient (log P_{ow})	9.029±0.917[a]
Partition Coefficient (log K_{oc})	6.29[a]

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Data from SciFinder originating from experimentally determined properties
c) Experimental data (Ou and Peng, 1999)

Known uses: Tris(tribromoneopentyl) phosphate is used as a flame retardant in polyurethanes and unsaturated polyesters (Ou and Peng, 1999).

Synonyms: 1-Propanol, 3-bromo-2,2-bis(bromomethyl)-, phosphate (3:1) (8CI,9CI); CR 900; FR 370; FR 372; Flame Cut 175; Flame Cut 175R; Kronitex PB 370; PB 370; Reoflam FR 370; TPB 3070; Tris[2,2-bis(bromomethyl)-3-bromopropyl] phosphate; Tris[3-bromo-2,2-bis(bromomethyl)propyl] phosphate

Human exposure: No data available.

Toxicity: No data available**.**

Eye/skin irritation: No data available.

Genotoxicity: No data available.

Endocrine effects: No data available.

Absorption, distribution and excretion: No data available.

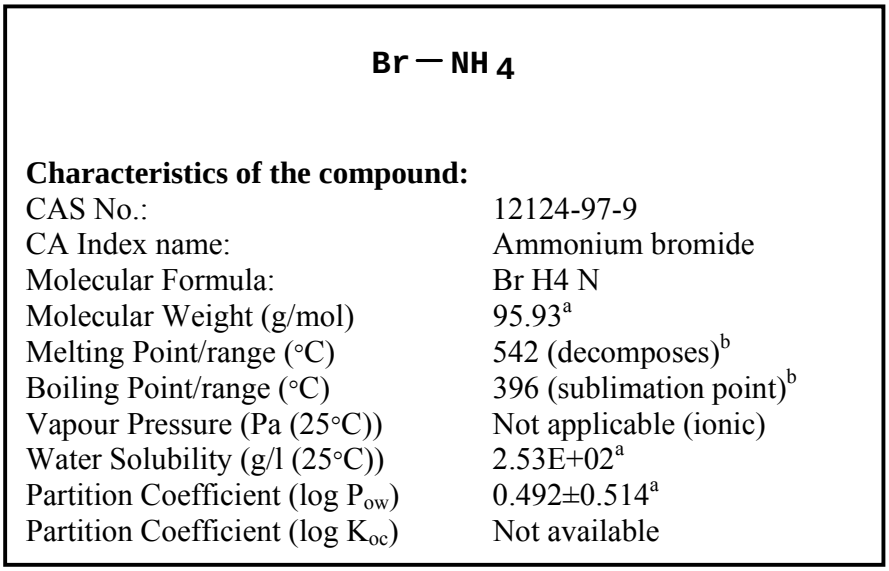
Bioaccumulation, degradation and fate: No data available.

Environmental levels: No available data.

Emissions and monitoring data in the Nordic countries: No data available

4.3 Inorganics

4.3.1.1 Ammoniumbromide



Characteristics of the compound:

CAS No.:	12124-97-9
CA Index name:	Ammonium bromide
Molecular Formula:	Br H4 N
Molecular Weight (g/mol)	95.93[a]
Melting Point/range (°C)	542 (decomposes)[b]
Boiling Point/range (°C)	396 (sublimation point)[b]
Vapour Pressure (Pa (25°C))	Not applicable (ionic)
Water Solubility (g/l (25°C))	2.53E+02[a]
Partition Coefficient (log P_{ow})	0.492±0.514[a]
Partition Coefficient (log K_{oc})	Not available

a) Data from SciFinder originating from calculated properties (ACD/labs Software V9.04)
b) Experimental data from the Handbook of Chemistry and Physics 77ed (CRC Press)

Known uses: Used as a flame retardant in fire-, insect-, and decay-resistant wood (Ishikawa et al.,). Used in some cases as a flame retardant component in water based flame extinguishing foams(Shiga,), used in process graving and lithography, corrosion inhibitor (metal treatment) (TOXNET, 2008). Ammoniumbromide is also use in bleaching solutions (photographic emulsions) for film development photographic processes (Lunar et al., 2004) and probably will be found in photographic waste waters.

Synonyms: Hydrobromic acid monoammoniate; Spectrum XD 3899

Human exposure: Bromide salts, should be considered to be moderately toxic: probable oral lethal dose (human) 0.5-5 g/kg for a 70 kg person (TOXNET, 2008).

Toxicity: Oral administration of ammoniumbromide in rat resulted in an LD_{50} of 2700 mg/kg with effects on sense organs and olfaction, behaivoural effects (somnolence and a general depressed activity), and on respiration. Another study on mouse reported an oral LD_{50} of 2860mg/kg with effects similar to rat. Intraperitoneal administration of ammoniumbromide in mouse gave an LD_{50} of 559 mg/kg and a similarly on guinea pig an LD_{50} of 535 mg/kg (RTECS, 2008).

Eye/skin irritation: No data available.

Genotoxicity: Ammonium bromide was tested for mutagenicity on the plant *Tradescantia Paludosa*. Results show that ammonium bromide gives a positive

response at a relatively high concentration of 1 mM. Results suggests that this compound may be a possible mutagen (Ma et al., 1984).

Endocrine effects: No data available.

Absorption, distribution and excretion: No data available.

Bioaccumulation, degradation and fate: No data available.

Environmental levels: No data available

Emissions and monitoring data in the Nordic countries: No data available

4.4 Concluding remarks

Limited data is available on toxicity, ecotoxicity, endocrine effects, and the absorption, distribution and excretion and bioaccumulation/concentration processes of these 21 "new" BFRs. For 1,4-Bis(pentabromophenoxy)tetrabromobenzene (CAS 58965-66-5), Pentabromobenzyl acrylate (CAS 59947-55-1) and Tris(tribromoneopentyl) phosphate (CAS 19186-97-1) there is no data available on any type of effect studies made or any reports on environmental concentrations. The only available data is calculated properties extracted from the SciFinder data base and additional properties (e.g. calculations in SPARC) that have been used for the long range transport assessment.

A perusal of the peer reviewed literature revealed that whereas some environmental effect data exist for many of the "new" BFRs, they often have not been found, or have not been analysed for, in environmental media. These include the following compounds: Tetrabromobisphenol A diallylether (CAS 25327-8-3), 2,4,6-Tris(2,4,6-tribromophenoxy)-1,3,5-triazine (CAS 25713-60-4). Also Benzene, ethenyl-, ar-bromo derivatives (CAS 125904-11-2), which is mostly dibromostyrene (CAS 31780-26-4) (additional monomers are the monobromostyrene and tribromostyrene), lacks any data on environmental levels and only a IUCLID report has been found, which is interesting but insufficient to serve for any valid risk assessment. As there are many different types of dibromostyrenes (variable positioning of the bromines) with different CAS numbers we cannot exclude that viable results on environmental effects and/or environmental levels may be available but finding those is not within the scope of this study. Similarly, CAS 77098-07-8, defined as a combination of the three compounds 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol, was identified by Abermarle Corporation and Great Lakes Chemical corporation as the BFR 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester (CAS 20566-35-2). The report that these corporations submitted to the US EPA HPV challenge program is the only available source of information on the potential environmental effects of this compound. Also under investigation is 1-Propanol, 2,2-dimethyl-, tribromoderivative (CAS 36483-57-5) which in the SciFinder database is represented by the Dibromoneopentyl alcohol (CAS 3296-90-0) and for which no data on environmental levels exist. Ethylene bistetrabromo phthalimide (CAS 32588-76-4), Tetrabromophthalic anhydride (CAS 632-79-1) and Ammoniumbromide (CAS 12124-97-9) was found to be devoid of any relevant data on environmental levels.

Only one, to our knowledge, relevant publication on Tetrabromobisphenol A bis(2,3-dibromopropylether) (CAS 21850-44-2) was found in the peer reviewed literature which reported the presence of this compound in dust samples after a flooding episode in Germany. More screening studies need to be performed on levels of this compound and other TBBPA derivatives in the domestic and workplace environments as well as in biota near potential sources to evaluate their persistence and long range transport and environmental impact.

Hexabromobenzene, pentabromotoluene , pentabromoethyl-benzene have been detected in a handful of studies: their presence has been reported in air and herring gull eggs from the Great Lakes region (USA), sediments in Japan and Germany, sewage sludge in Sweden and in glaucous gull eggs and plasma from the Norwegian Arctic. In addition, pentabromoethylbenzene has been found in the atmosphere of Chicago and in the UK. Most interesting is the recent findings of 2,4,6-tribromophenyl allyl ether in sewage sludge in Germany and in hooded and harp seal from the Barent sea which indicate that this compound is relatively persistent, bioaccumulates and is susceptible to long range transport to arctic regions. As these findings are quite recent more studies need to be performed to evaluate the behaviour of this compound in the food web and that threat it poses.

2,4,6-tribromophenol (TBP) has been detected in Australian biota and seems to be naturally occurring in algae, bryozoa, hydroids and sponges which makes it difficult to acertain the magnitude of antropogenic influence on concentrations found in vertebrates and top predators. TBP has also been found in river sediments from the Rhone estuary, in riverine and marine sediments in Japan, and in flue gas emissions from a hazardous waste incinerator in Sweden. In addition, both a health and risk assessment has been made for TBP based on data and predictions available at that time.

Decabromodiphenyl ethane (DBDPE) and 1,2-Bis(2,4,6-tribromophenoxy)-ethane (BTBPE) have generally been studied simultaneously as they are replacement compounds for the Penta-, Octa-, and DecaBDE mixtures. Like the PBDEs, they occur primarily bound to particles. They have been found in household dust and atmospheric particulate matter from the US and Sweden, in personal air monitoring devices of workers in an electronic waste facility in Sweden, in air from around the Great Lakes, and in tree bark from the Northeastern US. The detection, primarily of the more volatile BTBPE, in herring gull eggs from the Great Lakes and in the food chain of Lake Winnipeg, especially in predatory fish, proves that these compounds bioaccumulate to some degree. BTBPE have also been found in the Norwegian arctic (glaucous gull eggs), and in Northern fulmar eggs from the Faroe Island. Even if the concentrations are quite low, the results prove that the compounds are persistent and are transported to arctic regions. As their environmental behavior is similar to that of DecaBDE monitoring of these compounds should be considered to identify increasing trends in the environment and to screen the population for compounds that can be found in the domestic and work environment.

Bis(2-ethylhexyl)tetrabromophtalate has only recently been found in dust in the Boston area and in biosolids from a San Francisco WWTP. More data are needed, especially from biota and food web studies, to ascertain whether this compound is persistent and bioaccumulates in aquatic environments close to potential sources and urban areas.

5. Long range transport potential (LRTP) Assessment of Selected Brominated Flame Retardants

The long range transport behaviour of chemicals is one of the criteria which make a compound a persistent organic pollutant (POP). The long range transport potential of these 21 selected brominated flame retardants was estimated using model-based tools that are well established and readily available. These tools include:

- The calculation of transport (characteristic travel distance) and target-oriented (transport efficiency) long range transport indicators with the help of version 2.11 of the "The OECD POV and LRTP Screening Tool"., its purpose "is to estimate persistence and long-range transport potential of organic chemicals at a screening level, and to provide context for making comparative assessments of environmental hazard properties of different chemicals." (Scheringer et al., 2007). Accordingly, the LRTP indicators for the 22 substances were compared with those of substances with well established transport characteristics. The Monte Carlo functionality of the tool was used to assess the influence of the uncertainty of the chemical input parameters on the LRTP predictions.
- The concepts of the Arctic Contamination Potential (ACP) and the Arctic Contamination and Bioaccumulation Potental (ACBAP) as introduced by Wania (2006) and Czub et al. (2008). Based on their measured or – more likely - estimated distribution properties, the 21 flame retardants was placed on chemical space maps displaying the dependence of the ACP and ACBAP on the chemical partitioning and degradation properties. Again, a comparison of the indicators for the 21 substances with those for substances with well established transport characteristics was included.

5.1 Assessment of transport behaviour based on partitioning properties

In a first step, we assessed the likely LRT behaviour of the "new" BFR using only chemical distribution properties, i.e. ignoring the persistence of the compounds. We used the air-water partitioning coefficient K_{AW} and the octanol-air partitioning coefficient K_{OA} to locate the BFR chemicals in the chemical partitioning space defined by these two equilibrium partitioning coefficients. K_{AW} and K_{OA} were predicted with the SPARC On-line Calculator, which is a chemical property prediction software, which is available for public use, free of charge, and can be accessed at http://sparc.chem.uga.edu (Hilal et al., 2000). We then used previously published chemical space maps (Figure 2 to 4 (Wania, 2003;Wania, 2006;Czub et al., 2008)) that we overlaid with the BFRs to deduce something about their transport behaviour.

Table 5. Partitioning properties

CAS	Name	log K_{OA}	log K_{AW}
	1-Propanol, 2,2-dimethyl-, tribromo deriv.[a]		
36483-57-5	1-Propanol, 2,2-dimethyl-, tribromo deriv.	7.1	-4.28
1522-92-5	Tribromoneopentyl alcohol	7.6	-5.69
	Benzene, ethenyl-, ar-bromo deriv.[a]		
125904-11-2*	1,4 dibromo-2 ethynyl benzene (Dibromostyrene der.).	6.4	-1.90
31780-26-4	2,2-dibromoethenylbenzene (Dibromostyrene der.)	6.2	-1.62
2039-88-5	Benzene, 1-bromo-2-ethenyl (Monobromostyrene der)	5.1	-1.38
118-79-6	2,4,6-Tribromophenol	6.6	-2.30
19186-97-1	Tris(tribromoneopentyl) phosphate	15.0	-6.08
20566-35-2 or 77098-07-8	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester	18.8	-14.49
21850-44-2	Tetrabromobisphenol A bis(2,3-dibromopropyl ether)	21.0	-8.01
25327-89-3	Tetrabromobisphenol A diallyl ether	15.5	-4.43
26040-51-7	Bis(2-ethylhexyl) tetrabromophthalate	17.7	-5.95
3278-89-5	2,4,6-Tribromophenyl allyl ether	8.2	-2.41
3296-90-0	Dibromoneopentyl glycol	7.5	-7.66
37853-59-1	1,2-Bis(2,4,6-tribromophenoxy)ethane (BTBPE)	15.0	-5.17
56362017 or 25713-60-4	2,4,6-Tris(2,4,6-tribromophenoxy)-1,3,5 triazine	24.9	-11.43
58965-66-5 or 32588-76-4	Ethylene bis(tetrabromophthalimide) (EBTPI)	26.7	-9.06
59447-55-1	Pentabromobenzyl acrylate	11.7	-5.24
632-79-1	Tetrabromophtalic anhydride	11.8	-9.04
84852-53-9	Decabromodiphenylethane (DBDPE)	18.8	-6.29
85-22-3	Pentabromoethylbenzene	9.9	-2.92
87-82-1	Hexabromobenzene (HBB)	9.9	-3.03
87-83-2	Pentabromotoluene (PBT)	9.5	-3.00

a) The software SPARC and SciFinder has identified the following structures and properties for the listed cas.no.

5.2 Modes of (global) transport behaviour

Using the results of global transport simulations for a number of hypothetical chemical partitioning property combinations, Wania (2003, 2006) defined four modes of global transport behaviour for organic chemicals. These are:

- **Fliers:** Substances that are too volatile to partition appreciably into the surface compartments water and soil. These substances can have a very high LRT potential if they are resistant to degradation in the atmosphere. However, their high volatility also means that they generally are not bioaccumulating in foodchains. An example of a persistent flier are the chlorofluorocarbons (CFCs) or tetrachloromethane (Carbon tetrachloride).
- **Multihoppers:** Substances with intermediate volatility that have the potential to cycle between the atmosphere and the Earth's surface by repeated deposition and evaporation. Some exchange primarily with aquatic surface media, others with terrestrial compartments (soil/foliage), and yet others can exchange with all type of surface media. If sufficiently persistent in air and surface media, such substances have a very large potential to accumulate in polar regions. An example

of a persistent multihopper is hexachlorobenzene (HCB).

- **Single Hoppers:** Substances that are too involatile to re-evaporate after they have been deposited to the Earth's surface. These chemicals can still undergo LRT, if they are emitted into the atmosphere and are not deposited until they reach the remote region (e.g. when rapid atmospheric transport occurs during a period of no precipitation). An example for a persistent single hopper is octachlorodibenzo-*para*-dioxin (OCDD).
- **Swimmers:** Substances that are water soluble and therefore could undergo LRT in the oceans (and in rivers), if they are very persistent in the aqueous phase. An example of a persistent swimmer is perfluorooctanesulfonate (PFOS)

By comparing the estimated partitioning properties of the "new" BFR with the ranges of partitioning properties that define the four modes of global transport behaviour (Figure 2), we can speculate as to their likely transport characteristics.

Based on their partitioning properties five of the investigated BFR substances are likely to be able to readily exchange between the Earth's atmosphere and surface, in particular lakes and oceans (see Figure 2). In other words, they are multi-hoppers (Wania, 2006). These are the styrenes with one or two bromine substitutions (CAS 2039-88-5, 31780-26-4, 125904-11-2), 1,3,5-tribromo-2-(2-propenyloxy)-benzene (CAS 3278-89-5) and 2,4,6-tribromophenol (CAS 118-79-6). We should caution that the partitioning properties of the tribromophenol apply to the protonated form only. The estimated pK_a of 6.34 for this substance however suggests that it can occur in ionized form within the environmentally relevant pH-range, and it will therefore have a considerably lower log K_{AW} value than is indicated in the chemical space maps (indicated by the white arrow pointing downwards).

Three more substances have partitioning properties (log K_{AW} around -3, log K_{OA} around 9.5 to 10) that place them in the transition area between multiple and single hoppers. These are the highly brominated monoaromatic compounds pentabromoethylbenzene (CAS 85-22-3), pentabromotoluene (CAS 87-83-2), and hexabromobenzene (CAS 87-82-1).

Three substances are fairly volatile (log K_{OA} below 8), but are so water soluble that their log K_{AW} is low (log K_{AW} below -4). These are the brominated and hydroxylated neopentyl compounds, whereby the diol (3296-90-0) has a considerably lower log K_{AW} than the monoalcohols (CAS 36483-57-5 and 1522-92-5). They thus have the partitioning properties enabling transport in the aqueous phase ("swimmers"), i.e. could undergo long range transport in the atmosphere, if they are sufficiently resistant to degradation in water. The tribromophenol (CAS 118-79-6) in its protonated form also is a "swimmer".

Two substances have partitioning properties in a transition area, where the transport characteristics are poorly defined. These are pentabromobenzyl acrylate (CAS 59447-55-1) and Tetrabromophthalic anhydride (CAS 632-79-1).

Most of the remaining brominated flame retardants (CAS 19186-97-1, 20566-35-2 or 77098-07-8, 21850-44-2, 25327-89-

3, 26040-51-7, 37853-59-1, 56362017 or 25713-60-4, 58965-66-5 or 32588-76-4, 84852-53-9) are clearly too involatile (log K_{OA} > 15) to be present in the atmospheric gas phase. If they occur in the atmosphere at all, it is likely in the particulate form. The atmospheric transport behaviour of these so-called "single hoppers" is determined by the transport behaviour of the particle to which they sorb.

5.3 Arctic Contamination Potential (Wania, 2003;Wania, 2006)

Wania (2003, 2006) defined the Arctic Contamination Potential ACP as a quantitative measure of the potential of an organic substance to undergo global scale transport and accumulate in the Arctic environment. The ACP is thus an integrative indicator of long range transport potential. Calculated with the zonally averaged global transport and distribution model Globo-POP, it is defined as the fraction of the total cumulative global emissions of a substance that is present in the surface media of the Arctic zone after a given amount of time. In those calculations the zonal distribution of the emission is assumed to match the zonal distribution of the global human population. The $eACP_{10}^{air}$ is the Arctic Contamination Potential for a substance after 10 years of continuous emissions to the atmosphere. Wania (2003, 2006) calculated the $eACP_{10}^{air}$ for hypothetical chemicals of variable partitioning property combinations K_{AW} and K_{OA} and displayed the results as a function of the twodimensional chemical space defined by K_{AW} and K_{OA}. Figure 3 shows this chemical space plot for the $eACP_{10}^{air}$ of perfectly persistent chemicals.

By comparing the estimated partitioning properties of the "new" BFR with the ranges of partitioning properties that yield high $eACP_{10}^{air}$ values (Figure 3), we can speculate as to which BFRs would have a high propensity for accumulation in the Arctic, if they were persistent. Under the assumption of perfect persistence, the styrenes with one or two bromine substitutions would be expected to have a very high potential to reach the Arctic environment. Based on partitioning properties alone, 2,4,6-tribromophenyl allyl ether and protonated 2,4,6-tribromophenol would also be expected to have a high potential for long range transport to the Arctic. The highly brominated monoaromatics would also be able to reach the Arctic, albeit with a lower efficiency.

5.4 Arctic Contamination and Bioaccumulation Potential

Czub et al. (Czub et al., 2008) used a global transport model in combination with an Arctic human food chain accumulation model to constrain the partitioning properties of substances that are amenable to transport to the Arctic and accumulation through the Arctic human food chain. In particular, they defined the Arctic Contamination and Bioaccumulation Potential AC-BAP as the quotient of the human body burden of the chemical and the quantity of chemical cumulatively emitted to the global environment. It is thus the fraction of the total global emission amount that is present in one Arctic human being. The specific parameter $AC\text{-}BAP_{70}$ is based on the body burden in a 30 year old woman who was born 40 years after steady emission into the global environment began. This Inuit mother was exposed to the hypothetical contami-

nants entirely from seal blubber as part of the traditional marine diet, and was nursing her third child 50 days after its birth (Czub et al., 2008). Figure 4 shows the results and delineates in red the area of high AC-BAP_{70}, which means a high potential for becoming an Arctic contaminant based on partitioning characteristics. By comparing the estimated partitioning properties of the "new" BFR with the ranges of partitioning properties that yield high AC-BAP_{70} values (Figure 4), we can speculate as to which BFRs would have a high propensity for accumulation in the Arctic human food chain, if they were persistent.

Even though it was predicted to have partitioning properties that favour transport to the Arctic, the monobromostyrene (CAS 2039-88-5) is predicted to have a low AC-BAP_{70} by virtue of being too volatile for efficient bioaccumulation. The two dibromostyrenes, on the other hand, fall within the area of elevated AC-BAP_{70}, and clearly could be potential Arctic contaminants, if they are resistant to degradation in the environment and to biotransformation reactions in the organisms making up the food chain.

Although tribromophenol falls within the area of high AC-BAP_{70}, its deprotonated form would likely fall outside it, so its potential to become an arctic contaminant depends not only on its resistance to transformation, but also on the pH of the water relative to its pK_a of 6.34. At the pH of sea water, most of tribromophenol would be expected to be ionized.

The brominated and hydroxylated neopentyl compounds are too water soluble to be subject to efficient bioaccumulation, so even though they may have the partitioning properties for efficient LRT in the oceans, they are unlikely to enter the food chain to a significant extent.

2,4,6-tribromophenyl allyl ether (CAS 3278-89-5) is close to the "bull's eye" of the AC-BAP_{70} plot and thus has predicted partitioning properties that make it exceptionally susceptible to becoming an Arctic contaminant. This clearly indicates a need to establish its environmental persistence and suscep-tibility to metabolic transformation.

The three highly brominated monoaromatics (pentabromoethylbenzene CAS 85-22-3, pentabromotoluene CAS 87-83-2, hexabromobenzene CAS 87-82-1) fall within or very close to the area of high AC-BAP_{70} and in particular have partitioning properties very similar to many known Arctic contaminants (e.g. PCBs). Again, the potential for degradation in the physical environment and in organisms will need to be established to assess the potential of these substances to become Arctic contaminants.

Although outside of the red outline in Figure 3, 2-Propenoic acid, (2,3,4,5,6-pentabromophenyl)-methyl ester (CAS 59447-55-1) have partitioning properties not unlike many known Arctic contaminants (for detailed discussion of this apparent contradiction see (Czub et al., 2008) and could therefore have some potential to become Arctic contaminants, if sufficiently persistent. This is likely not the case for 4,5,6,7-tetrabromo-1,3-isobenzofurandione (CAS 632-79-1), which has a log K_{OW} too low for efficient bioaccumulation.

The remaining substances have a much larger molecular size and a much lower volatility than substances that typically believed to have the potential to become Arctic contaminants.

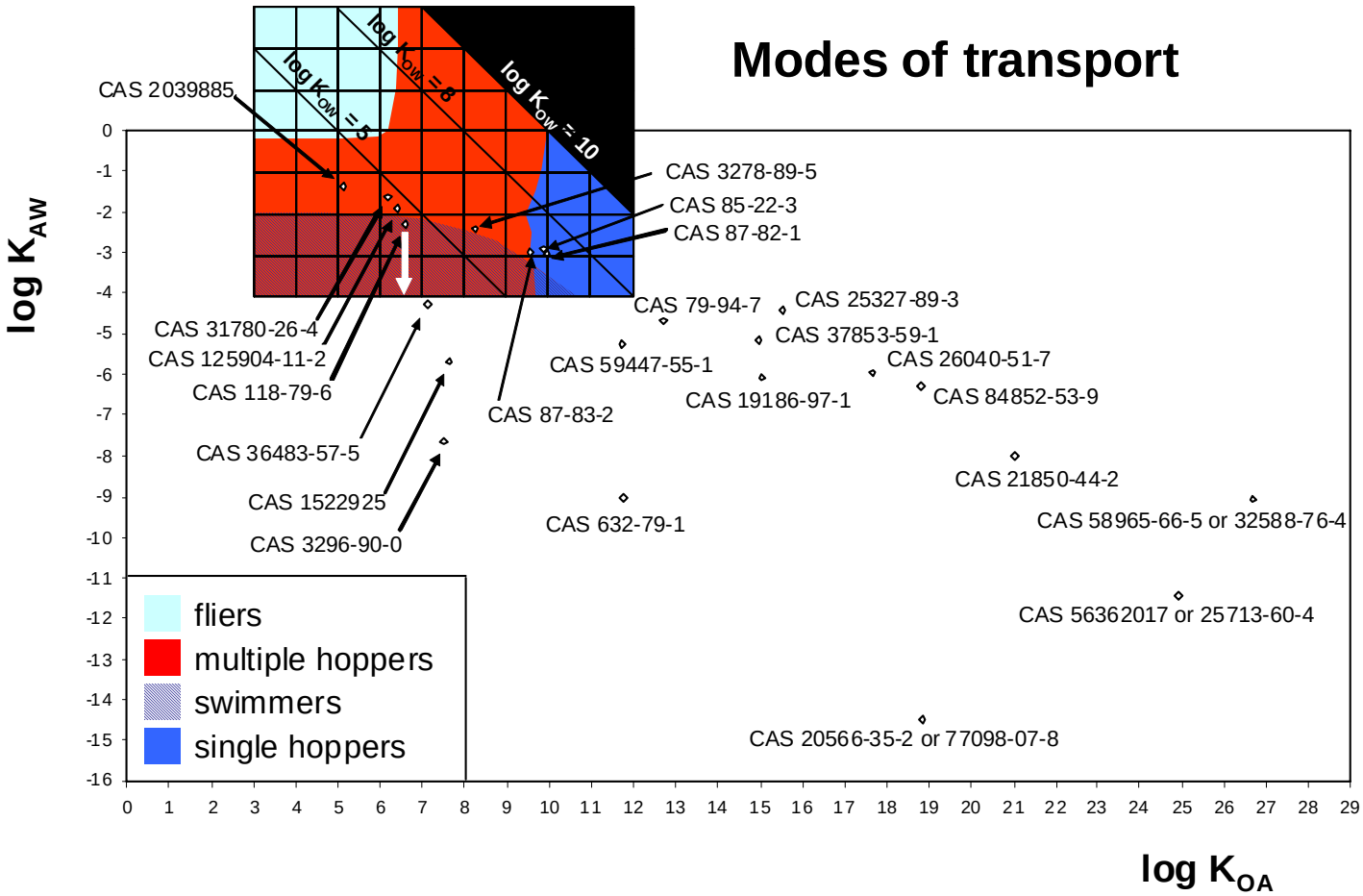


Figure 2. Estimated partitioning properties K_{AW} and K_{OA} of "new" BFR substances relative to the ranges of partitioning properties delineating the four major modes of global transport as established by Wania (2003, 2006). The modes of transport are not indicated for large parts of the chemical space, because no global transport simulations were conducted for substances with log K_{AW} < -4 and log K_{OA} > 12. Substances with log K_{OA} > 12 are likely to be "single hoppers", whereas those with a log K_{AW} < -4 are "swimmers".

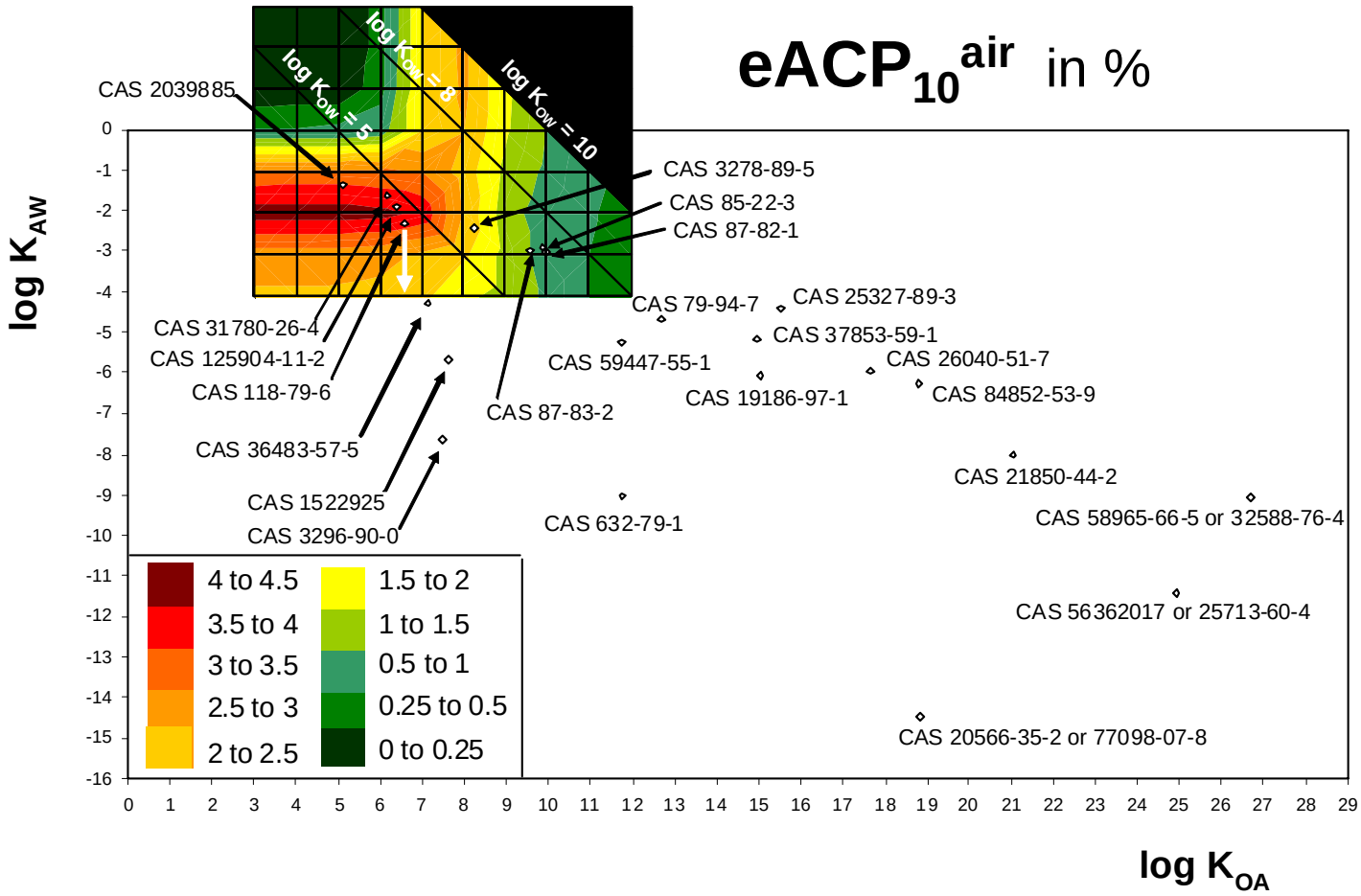


Figure 3. Estimated partitioning properties K_{AW} and K_{OA} of "new" BFR substances relative to the ranges of partitioning properties that yield high Arctic contamination potential $eACP_{10}^{air}$, as defined in Wania (2003, 2006). The $eACP_{10}^{air}$ values are not indicated for large parts of the chemical space, because no global transport simulations were conducted for substances with log K_{AW} < -4 and log K_{OA} > 12.

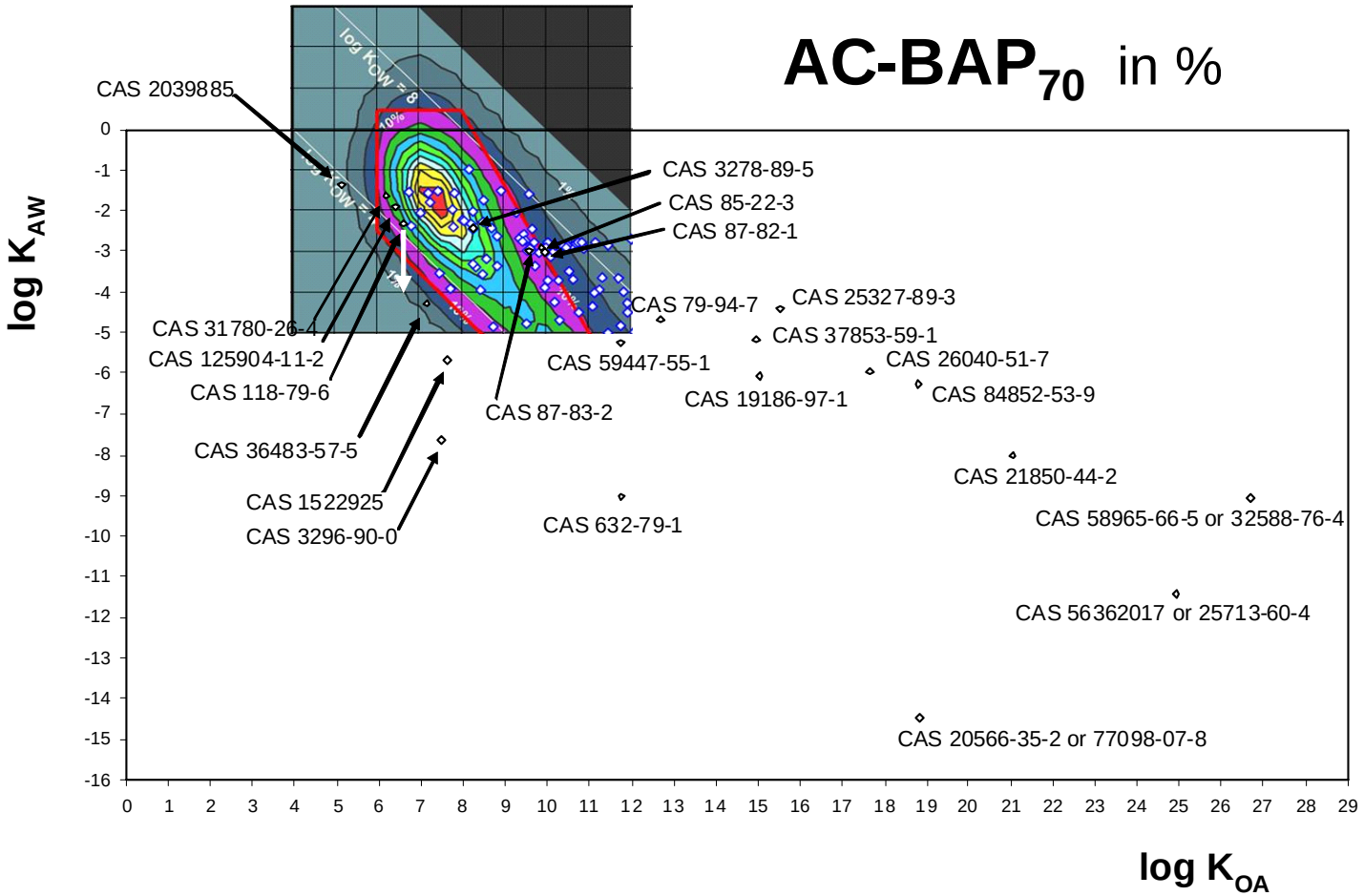


Figure 4. Estimated partitioning properties K_{AW} and K_{OA} of "new" BFR substances relative to the ranges of partitioning properties that yield high Arctic Contamination and Bioaccumulation Potential AC-BAP$_{70}$, as defined in Czub et al. (2008). The AC-BAP$_{70}$ values are not indicated for large parts of the chemical space, because no global transport simulations were conducted for substances with log K_{AW} < -5 and log K_{OA} > 12. The red outline indicates the area of highest estimated AC-BAP$_{70}$.

Table 6. Calculated physicochemical properties and degradation half-lifes in air, water and soil.Compounds marked have fairly extreme partitioning, properties that are deemed to lie outside of the domain of applicability of the model.

CAS. no.	Chemical Name	Molar Mass (g/mol)	Log K_{AW}	Log K_{OW}	Half-life in air (hours)	Half-life in water (hours)	Half-life in soil (hours)
	1-Propanol, 2,2-dimethyl-, tribromo deriv.						
36483-57-5	1-Propanol, 2,2-dimethyl-, tribromo deriv.	324.8	-4.28	2.6	25	900	1800
1522-92-5	Tribromoneopentyl alcohol	324.8	-5.69	1.8	50.1	900	1800
	Benzene, ethenyl-, ar-bromo derivatives						
125904-11-2	1,4 dibromo-2 ethynyl benzene (Dibromostyrene der.).	261.9	-1.90	4.2	4.7	900	1800
31780-26-4	2,2-dibromoethenylbenzene (Dibromostyrene der.)	261.9	-1.62	4.26	16.6	900	1800
2039-88-5	Benzene, 1-bromo-2-ethenyl (Monobromostyrene der)	183.0	-1.38	3.47	5.46	900	1800
118-79-6	2,4,6-Tribromophenol	330.8	-2.30	4.0	270.3	1440	2880
19186-97-1	Tris(tribromoneopentyl) phosphate	1020.0	-6.08	8.2	1.7	4320	8640
20566-35-2 or 77098-07-8	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester	627.91	-14.49	4.53	4.2	1440	2880
21850-44-2	Tetrabromobisphenol A bis(2,3-dibromopropyl ether)	943.6	-8.01	12.12	12.2	4320	8640
25327-89-3	Tetrabromobisphenol A diallyl ether	624.0	-4.43	10.4	1.9	4320	8640
26040-51-7	Bis(2-ethylhexyl) tetrabromophthalate	706.1	-5.95	10.93	5.9	1440	2880
3278-89-5	2,4,6-Tribromophenyl allyl ether	370.9	-2.41	5.4	4	1440	2880
3296-90-0	Dibromoneopentyl glycol	261.9	-7.66	0.1	14.3	360	720
37853-59-1	1,2-Bis(2,4,6-tribromophenoxy)ethane (BTBPE)	687.6	-5.17	9.1	8.6	4320	8640
56362-01-7 or 25713-60-4	2,4,6-Tris(2,4,6-tribromophenoxy)-1,3,5 triazine	1067.4	-11.43	12.55	86.7	4320	8640
58965-66-5 or 32588-76-4	Ethylene bis(tetrabromophthalimide) (EBTPI)	1366.9	-9.06	16.39	2351	4320	8640
59447-55-1	Pentabromobenzyl acrylate	556.7	-5.24	6.0	11.9	4320	8640
632-79-1	Tetrabromophtalic anhydride	463.7	-9.04	2.6	5261	4320	8640
84852-53-9	Decabromodiphenylethane (DBDPE)	971.2	-6.29	11.64	53.6	4320	8640
85-22-3	Pentabromoethylbenzene	500.6	-2.92	6.4	111.6	4320	8640
87-82-1	Hexabromobenzene (HBB)	551.5	-3.03	6.4	11162	4320	8640
87-83-2	Pentabromotoluene (PBT)	486.6	-3.0	6.1	693.8	4320	8640

5.5 Assessment of Transport Behaviour Using the OECD Pov& LRTP Screening Tool

In the last decade a number of research groups have developed model-based tools for the assessment of an organic chemical's persistence and long range transport potential. In particular, a variety of quantitative indicators for the LRTP have been proposed. Under the auspices of the OECD, several of these models and indicators have been compared and have been found to give largely consistent results (Fenner et al., 2005). To simplify and encourage the use of models in the assessment of overall persistence and LRTP, a consensus model emerged from the work under the auspices of the OECD. This consensus model is the OECD Pov & LRTP Screening Tool by Wegmann et al. (Wegmann et al., 2009) ("The Tool").

We used "The Tool" to estimate an overall persistence P_{OV} and two different measures of long range transport potential (LRTP), namely the characteristic travel distance in km (CTD) and the transfer efficiency in % (TE). The Tool also allows a comparison with "thresholds" of P_{OV} and LRTP, which are derived from known persistent organic pollutants (POPs).

Table 6 lists the input parameters that were supplied to the Tool. The partitioning properties log K_{AW} and log K_{OW} were estimated using SPARC On-Line calculator, and the degradation half-lifes were estimated using the EPISuite. For seven substances the Tool displayed a warning (orange background in Table 6): these substances have fairly extreme partitioning properties (log K_{OW} > 10, log K_{AW} < -10) that are deemed to lie outside of the domain of applicability of the model. The model can still calculate a P_{OV} and LRTP parameters for those substances, but they should be interpreted with caution.

The results for the overall persistence are given in Table 7, those for the characteristic travel distance in Table 8, and those for the transfer efficiency in Table 9. The latter two tables also include information on the estimated particle bound-fraction of the chemical in the atmosphere (Φ_{Air}). Φ_{Air} is an important parameter in controlling the potential for atmospheric LRT, because it influences the rates of deposition and atmospheric degradation. In particular, particle-bound substances tend to be deposited quite rapidly as a result of dry and wet deposition processes. On the other hand, the models typically assume that a particle-bound substance is less likely to react with photo-oxidants.

Several BFR, in particular those which sorb entirely to particles in the atmosphere (Φ_{Air} = 1) have CTDs around 2860 km and TE of around 12.7 %. This is because this is the CTD and TE of atmospheric particles in "The Tool". Atmospheric degradation half lifes supplied to the model have no bearing on the results for these substances because particle-bound substances are assumed to not undergo reactions with photo-oxidants. One substance (CAS 20566-35-2 or 77098-07-8) with Φ_{Air} = 1 has a CTD and a TE much lower than this threshold (233 km, 1 %), which is likely the result of an exceptionally low log K_{AW} value (log K_{AW} = -14.5), which leads the model to predict erroneously fast wash-out rates of the tiny fractions of this chemicals predicted to be in the atmospheric gas phase.

Only three substances are predicted to have CTDs that exceed this benchmark

set by particle transport: 11,000 km for hexabromobenzene (87-82-1), 6900 km for pentabromotoluene (87-83-2), and 4850 km for tribromophenol (118-79-6). Only the former two have TE values that exceed the threshold for particles.

These CTD and TE values probably overestimate the LRTP of those three chemicals, because they neglect the possibility of direct photolysis of brominated substances, which is not included in the atmospheric degradation rate estimation in EPISuite. Photolytic debromination may be particularly relevant for highly brominated aromatic substances. The CTD of tribromophenol is likely further overestimated, because the deprotonated form would have a much lower log K_{AW} than the protonated form and would therefore by subject to much more efficient rain scavenging. Acid rain would be less effective in scavenging this compound than rain with neutral pH.

Figure 5 displays the results of the Tool for the brominated flame retardants relative to thresholds obtained from the P_{OV} and LRTP of established POPs (Klasmeier et al., 2006). In the panel to the left the CTD is the LRTP indicator, whereas in that on the right the TE is used. In either case, the x-axis is the P_{OV}.

Only two chemicals fall in the quadrant to the upper right, indicative of substances that are as persistent and as subject to LRTP as known POPs, in both plots in Figure 5: hexabromobenzene (87-82-1) and for pentabromotoluene (87-83-2). If TE is used as the LRTP indicator, most of the entirely particle-bound substances have a LRTP estimate above the POP threshold, even though the CTD estimate for those same chemicals is below the POPs threshold.

5.6 Summary of the LRTP Assessment

The potential for these selected BFRs to be subjected to long range transport (LRT) was studied. Results showed that dibrominated styrenes (CAS 31780-26-4, 125904-11-2), 2,4,6-tribromophenyl allyl ether (CAS 3278-89-5) and pentabromobenzyl acrylate (CAS 59447-55-1) - based on their partitioning properties alone - were judged to have the potential to undergo LRT. However, estimated short atmospheric half life, based on the EPISuite predictions, indicates that they are more likely to pose a problem in the near source environment, especially if they should be recalcitrant to biotransformation. Even if the predictions suggests 2,4,6-tribromophenyl allyl ether to have short atmospheric half life, recent findings of the detection of 2,4,6-tribromophenyl allyl ether in seal from the Barents Sea (Von Recke and Vetter, 2007) might suggest this compound, still, to be a possible concern, especially if levels in the arctic increases. Also, a valid concern is whether pentabromobenzyl acrylate may form a persistent and potentially bioaccumulative metabolite.

Table 7. Overall persistence values in days for brominated flame retardants estimated with the Tool using physical chemical partitioning properties estimated by SPARC and degradation half-lifes estimated by EPISuite.

CAS. No.	Chemical name	P_{OV}	P_{OV} Emission to air	P_{OV} Emission to water	P_{OV} Emission to soil
	1-Propanol, 2,2-dimethyl-, tribromo deriv.				
36483-57-5	1-Propanol, 2,2-dimethyl-, tribromo deriv.	91	8	53	91
1522-92-5	Tribromoneopentyl alcohol	77	28	4	77
	Benzene, ethenyl-, ar-bromo deriv.				
125904-11-2	1,4 dibromo-2 ethynyl benzene (Dibro-mostyrene der.).	95	0	40	95
31780-26-4	2,2-dibromoethenylbenzene (Dibromosty-rene der.)	91	1	40	91
2039-88-5	Benzene, 1-bromo-2-ethenyl (Monobro-mostyrene der)	40	0	39	40
118-79-6	2,4,6-Tribromophenol	154	26	66	154
19186-97-1	Tris(tribromoneopentyl) phosphate	519	382	260	519
20566-35-2 or 77098-07-8	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester	172	112	87	172
21850-44-2	Tetrabromobisphenol A bis(2,3-dibromopropyl ether)	519	432	260	519
25327-89-3	Tetrabromobisphenol A diallyl ether	519	421	260	519
26040-51-7	Bis(2-ethylhexyl) tetrabromophthalate	173	137	87	173
3278-89-5	2,4,6-Tribromophenyl allyl ether	168	1	58	168
3296-90-0	Dibromoneopentyl glycol	31	23	22	31
37853-59-1	1,2-Bis(2,4,6-tribromophenoxy)ethane	519	423	260	519
56362017 or 25713-60-4	2,4,6-Tris(2,4,6-tribromophenoxy)-1,3,5 triazine	519	432	260	519
58965-66-5 or 32588-76-4	Ethylene bis(tetrabromophthalimide)	519	432	260	519
59447-55-1	Pentabromobenzyl acrylate	518	59	258	518
632-79-1	Tetrabromophtalic anhydride	372	291	260	372
84852-53-9	Decabromodiphenylethane	519	432	260	519
85-22-3	Pentabromoethylbenzene	515	40	156	515
87-82-1	Hexabromobenzene	517	305	277	517
87-83-2	Pentabromotoluene	514	157	213	514

Table 8. Characteristic travel distance (CTD) in km and the estimated particle bound-fraction in the atmosphere (Φ_{Air}) for brominated flame retardants estimated with The Tool using physical chemical partitioning properties estimated by SPARC and degradation half-lifes estimated by EPISuite.

CAS. No.	Chemical name	CTD	CTD air	CTD water	Φ_{Air}
	1-Propanol, 2,2-dimethyl-, tribromo deriv.				
36483-57-5	1-Propanol, 2,2-dimethyl-, tribromo deriv.	459	459	92	6.7E-05
1522-92-5	Tribromoneopentyl alcohol	570	570	93	2.7E-04
	Benzene, ethenyl-, ar-bromo deriv.				
125904-11-2	1,4 dibromo-2 ethynyl benzene (Dibro-mostyrene der.).	98	98	69	9.5E-06
31780-26-4	2,2-dibromoethenylbenzene (Dibromosty-rene der.)	344	344	68	6.3E-06
2039-88-5	Benzene, 1-bromo-2-ethenyl (Monobro-mostyrene der)	113	113	68	5.9E-07
118-79-6	2,4,6-Tribromophenol	4850	4850	105	1.7E-05
19186-97-1	Tris(tribromoneopentyl) phosphate	2703	2703	135	1.00
20566-35-2 or 77098-07-8	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester	233	233	149	1.00
21850-44-2	Tetrabromobisphenol A bis(2,3-dibromopropyl ether)	2861	2861	121	1.00
25327-89-3	Tetrabromobisphenol A diallyl ether	2826	2826	121	1.00
26040-51-7	Bis(2-ethylhexyl) tetrabromophthalate	2861	2861	79	1.00
3278-89-5	2,4,6-Tribromophenyl allyl ether	100	83	100	5.8E-04
3296-90-0	Dibromoneopentyl glycol	37	18	37	5.1E-04
37853-59-1	1,2-Bis(2,4,6-tribromophenoxy)ethane	2833	2833	123	1.00
56362017 or 25713-60-4	2,4,6-Tris(2,4,6-tribromophenoxy)-1,3,5 triazine	2861	2861	121	1.00
58965-66-5 or 32588-76-4	Ethylene bis(tetrabromophthalimide)	2861	2861	121	1.00
59447-55-1	Pentabromobenzyl acrylate	499	499	398	0.60
632-79-1	Tetrabromophtalic anhydride	446	4	446	0.79
84852-53-9	Decabromodiphenylethane	2861	2861	121	1.00
85-22-3	Pentabromoethylbenzene	2014	2014	224	0.019
87-82-1	Hexabromobenzene	11008	11008	337	0.023
87-83-2	Pentabromotoluene	6937	6937	306	0.010

Table 9. Transfer efficiency in % for brominated flame retardants estimated with the Tool using physical chemical partitioning properties estimated by SPARC and degradation half-lifes estimated by EPISuite

CAS. no.	Chemical Name	TE	TE Emission to air	TE Emission to water	TE Emission to soil	Φ_{Air}
	1-Propanol, 2,2-dimethyl-, tribromo deriv.					
36483-57-5	1-Propanol, 2,2-dimethyl-, tribromo deriv.	0.24	0.24	8.7E-05	9.4E-04	6.7E-05
1522-92-5	Tribromoneopentyl alcohol	1.15	1.15	7.2E-07	6.0E-04	2.7E-04
	Benzene, ethenyl-, ar-bromo deriv.					
125904-11-2	1,4 dibromo-2 ethynyl benzene (Dibromostyrene der.).	7.9E-04	7.8E-04	5.4E-05	1.0E-05	9.5E-06
31780-26-4	2,2-dibromoethenylbenzene (Dibromostyrene der.)	5.3E-03	5.2E-03	3.9E-04	1.2E-04	6.3E-06
2039-88-5	Benzene, 1-bromo-2-ethenyl (Monobromostyrene der)	3.4E-04	3.4E-04	2.5E-05	1.3E-04	5.9E-07
118-79-6	2,4,6-Tribromophenol	4.32	4.32	0.50	6.4E-02	1.7E-05
19186-97-1	Tris(tribromoneopentyl) phosphate	11.3	11.3	5.1E-08	2.5E-12	1.00
20566-35-2 or 77098-07-8	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester	1.03	1.03	4.1E-24	2.4E-25	1.00
21850-44-2	Tetrabromobisphenol A bis(2,3-dibromopropyl ether)	12.7	12.7	1.0E-19	4.9E-24	1.00
25327-89-3	Tetrabromobisphenol A diallyl ether	12.4	12.4	3.5E-09	1.7E-13	1.00
26040-51-7	Bis(2-ethylhexyl) tetrabromophthalate	12.7	12.7	1.3E-13	8.6E-19	1.00
3278-89-5	2,4,6-Tribromophenyl allyl ether	1.6E-03	1.6E-03	1.7E-04	1.1E-06	5.8E-04
3296-90-0	Dibromoneopentyl glycol	0.076	0.076	9.0E-13	7.2E-09	5.1E-04
37853-59-1	1,2-Bis(2,4,6-tribromophenoxy)ethane	12.4	12.4	4.7E-08	2.2E-12	1.00
56362017 or 25713-60-4	2,4,6-Tris(2,4,6-tribromophenoxy)-1,3,5 triazine	12.7	12.7	2.0E-27	9.4E-32	1.00

The substances that have partitioning properties that suggests LRT and are predicted to be fairly persistent are the highly brominated monoaromatics, such as hexabromobenzene (CAS 87-82-1), pentabromotoluene (CAS 87-83-2), and pentabromoethylbenzene (CAS 85-22-3). The predicted LRT behaviour is comparable to those of established POPs, although these predictions may be overestimated because the LRT assessment does not include the possibility of photolytic debromination.

Some of the heavier BFRs, such as Decabromodiphenylethane (CAS 84852-53-9), have structures not unlike those of decaBDE, and may be subject to similar long range transport and bioaccumulation processes.

5.7 Sampling and analysis of new brominated flame retardants

5.8 Introduction

Quantitative and qualitative analyses of BFRs require the dissolution of the compounds in question in an extractive medium. Reactive FR types are copolymerized into the backbone of the polymer, and so are largely inaccessible to extraction. Additively applied flame retardants are more easily separated from the original polymer matrix. Therefore, the separation, detection and quantification by GC or LC can be applied. Which analytical method will be chosen depends strongly on the objective of the investigation. In thefollowing several approaches to analyse BFRs are introduced: Analyses of BFR treated products.

5.8.1 Test methods for elemental bromine

Sample pretreatment followed by gas chromategraphy - mass spectrometry (GC-MS) is perhaps the most widely used instrumental analysis technique used to distinguish restricted from non-restricted BFRs and for their quantification. This approach, however, is time consuming, requires destruction of the sample and has a relatively high analysis cost associated with the purchase and maintenance of the GC-MS equipment and the high level of expertise needed to operate it. It follows then that GC-MS testing might logically be implemented to determine whether a restricted BFR is present (and in what amount) only after a simpler "screening" test could first demonstrate the potential presence (or absence) of any BRF's or of bromine itself.

Energy dispersive X-ray fluorescence spectrometry (ED-XRF) is possibly the most commonly used analytical technique for screening of restricted substances, largely because of the significant speed advantage it has over traditional analysis methods and it's ability to be used with little or no sample pretreatment. The more sophisticated wavelength dispersive x-Ray (WD-XRF) units are not as commonly employed for this purpose due to the higher cost and expertise of operation associated with this instrument. In its simplest form, XRF analysis can provide both qualitative and semi-quantitative non-destructive elemental analysis (including bromine) in a start to finish time frame of several minutes. This is in contrast to the many hours typically needed for instrumental techniques requiring destructive sample pre-treatment (e.g. solvent extraction – GC/MS). Many users in the electrical and electronic industry supply chain are employing XRF as a screening tool to reduce the time and cost associated with the evaluation of RoHS compliance.

The use of XRF for the detection of halogens including bromine has been reported and plastics standard materials for this analysis are available (Riess et al., 2000). Assuming that the levels of detection are appropriate, a user may deduce that the absence of elemental bromine detection by XRF in a polymeric material, for instance, is sufficient evidence that a BFR of concern (e.g. PBB or PBDE) is not present. If detected, the user could establish a go/no-go quantity related to the regulation trigger level. Measurements below the trigger level could be deemed to be in compliance. If the XRF screening does detect elemental bromine at levels of concern, analysis using sample pre-treatment and GC-MS

analysis could be carried out to determine whether restricted BFRs are actually present and at what concentrations.
The use of infrared analysis as a way to determine if specific BFRs are present at intentionally added levels can also be considered. Generally, BFRs are used at the 5 - 20% level by weight in flame retarded polymer formulations. At this level, the characteristic absorbance bands of specific BFRs can be observed in the spectrum generated by a modern Fourier Transform Infrared (FTIR) spectrophotometer. As with XRF, an FTIR equipped with an attenuated total reflectance (ATR) accessory can analyze samples non-destructively in a few minutes. The spectra of some polymer resins and or their formulation additives can, however, interfere with the absorbance bands of BFRs, making identify-cation difficult at these concentrations. The use of non-destructive FTIR to detect BFRs at contaminant or non-intentionally added levels is not recommended due to the likely overwhelming spectral responses of the polymer formulation.
At least one report has suggested that Raman spectroscopy is less prone to matrix interference effects than infrared analysis and therefore better suited for rapid non-destructive analysis of BFRs in the acrylonitrile butadiene styrene (ABS) polymer. This study included identification of HBCDD, TBBPA and DecaBDE.

5.8.2 Analysis methods based upon pyrolysis or thermal desorption

Quantitative and qualitative analyses of BFRs require the dissolution of the compounds in question in an extractive medium. Reactive FR types are copolymerized into the backbone of the polymer, and so are largely inaccessible to extraction. Additively applied flame retardants are not easily separated from the original polymer matrix. Therefore, the separation, detection and quantification by GC or LC may be difficult to achieve. Pyrolysis–gas chromatography (Py–GC) is one of the techniques that can be used in these circumstances. Py-GC uses thermal energy (pyrolysis) to break down a polymeric chain followed by the separation of pyrolysates with GC with subsequent detection using a mass spectrometer.
Because of the large number of pyrolysates produced during the pyrolysis of polymer matrix with flame retardants, interpretation and identification of all components can be challenging. The typical isomer pattern of bromine can be used to identify brominated compounds in the gas chromatogram. Atomic emission detection (AED) can be used as an alternative to MS for the detection of specific –element containing fragments and their relative intensity pattern.
Riess et al. investigated technical flame retardants in polymers originating from electronic waste using an automated Curie-point pyrolysis system. The Curie-point pyrolysis system was directly connected to the split– splitless injector of a GC-MS system. It enables the characterization of thermoplastic styrene-based polymers containing brominated flame retardant additives, as well as the characterization of duroplastic polymers with reactive flame retardants embedded in the polymer matrix (Riess et al., 2000).

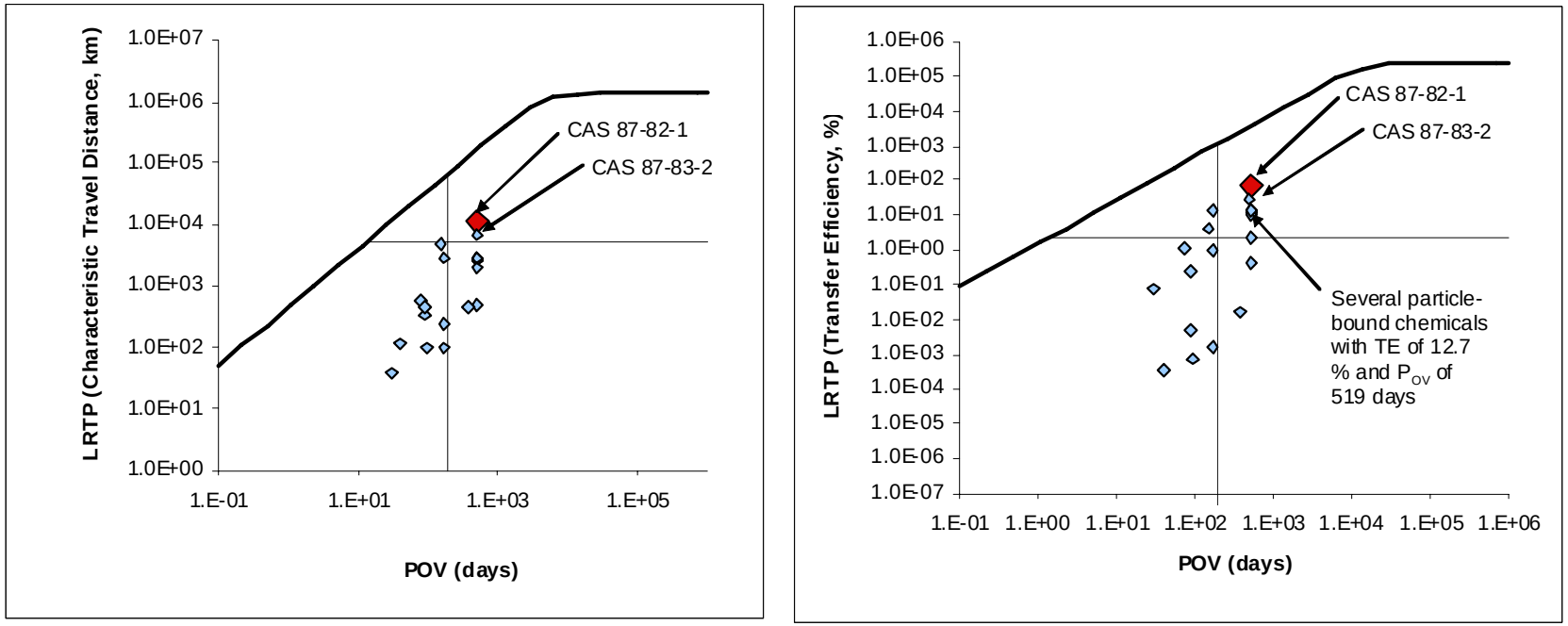


Figure 5. Results of "the Tool" for the brominated flame retardants relative to thresholds obtained from the P_{OV} and LRTP of established POPs (Klasmeier et al., 2006). In the panel to the left the CTD is the LRTP indicator, whereas in that on the right the TE is used. In either case, the x-axis is the P_{OV}.

5.9 Environmental samples

The objective of the analyses of environmental samples often is the detection of trace amounts of anthropogenic pollutant. Different methods need to be applied with respect to the chemical structure of the compounds of interest. Phenolic compounds like 2,4,6-tribromophenol or the TBBP-A derivatives are more hydrophilic opposite to the aromatic compounds and a different approach for chemical analyses is needed(see chapter 4.1.2.4).

Table 10. Neutral compounds

Substance Name	CAS No
Tetrabromobisphenol A bis(2,3-dibromopropyl `	21850-44-2
Tetrabromobisphenol A diallyl ether	25327-89-3
Hexabromobenzene (HBB)	87-82-1
Pentabromotoluene (PBT)	87-83-2
Pentabromoethylbenzene (PBEB)	85-22-3
2,4,6-Tribromophenyl allyl ether	3278-89-5
Decabromodiphenylethane (DBDPE)	84852-53-9
1,2-Bis(2,4,6-tribromophenoxy)ethane (BTBPE)	37853-59-1
1,4-Bis(pentabromophenoxy)tetrabromobenzene	58965-66-5
2,4,6-Tris(2,4,6-tribromophenoxy)-1,3,5 triazine	25713-60-4
Dibromostyrene (DBS)	125904-11-2
Pentabromobenzyl acrylate	59447-55-1
Ethylene bis(tetrabromophthalimide) (EBTPI)	32588-76-4
Tetrabromophtalic anhydride	632-79-1
Bis(2-ethylhexyl) tetrabromophthalate (TBPH)	26040-51-7
Tris(tribromoneophentyl)phosphate	19186-97-1

Extraction and Cleanup. Analytical procedures employed for the extraction and cleanup of neutral aromatic brominated compounds in biota like plasma and tissue samples can be based on methods developed for current-use BFRs. Several methods are described in the literature and can be easily adapted (for example Verrault, 2007). In general they base on extracting the biological sample with an apolar organic solvent and several clean-up and concentrations steps prior analysis and quantification by GC/MS.

Other samples types might require different extraction methods, like accelerated solvent extraction (ASE), soxhlet and ultrasonic extraction with various solvent types and system parameters optimised for the best possible performance (e.g. extraction cycle s, time, and temperature).

However, adequate method adaptation relies on the availability of commercial

reference standards. If standard compounds are not available only screening exercises are possible which base on the assumption that the analytical method for current-use BFR is applicable according to the similarity in chemical-physical properties and chemical structure. However, eventual losses during the analytical procedure cannot be uncovered and the compound of interest might not detectable without a prior validation of the method for new BFRs.

Bis(2-ethylhexyl) tetrabromophthalate (TBPH) and 2-ethylhexyl 2,3,4,5-tetrabromobenzoate (TBB) belong to the group of brominated phthalates which can be analysed in solids by using pressurized fluid extraction (3X with 100% dichloromethane at a temperature of 100°C and at 1500 psi) (Stapleton et al. 2008. Alternate and New Brominated Flame Retardants Detected in US House Dust. 10th Annual Workshop on Brominated Flame Retardants, Victoria, BC, Canada.).

1,2-Bis(tetrabromophthalimido)ethane and ethylene bis(tetrabromophthalimide) (EBTPI) might be analysed applying a modified method as well.

Analysis and quantification. Neutral brominated aromatic compound quantification can be performed using a gas chromatograph-mass spectrometer (GC-MS) operating in the electron capture negative ionization (ECNI) mode. The GC-MS(ECNI) analyte determination can be accomplished in the selected ion-monitoring (SIM) mode for the isotopic bromine anions 79Br- and 81Br-. Alternatively, a GC-highresolution MS in the electron ionization (EI) mode (GC-HRMS(EI)) can be applied. The GC-HRMS(EI) uses a MS system with a double focusing-magnetic sector mass analyzer operating at a mass resolution of 10 000 or greater with helium as a carrier gas. A total of four to eight ions, which consisted of the most abundant fragment anions and molecular ion clusters, can be monitored using SIM for HBB, BTBPE, PBEB, and PBT.

Brominated phthalate extracts can be analyzed using GC/ECNI-MS. TBB can be quantified using ion fragments (m/z) 357 (Quantitative) and 471 (Qualitative) while TBPH can be quantified using ion fragments (m/z) 463 (Quantitative) and 515 (Qualitative).

If volatilisation in GC cannot achieved without breakdown of the compounds of interest LC/MS methods can be applied as well.

However, due to the probable lack of commercially available standard compounds quantification of new BFRs can only be carried out by applying response factors of structurally similar chemicals. That will lead to semi-quantitative results biased by an elevated uncertainty. If no chemical with similar chemical structure is available either, only qualitative information can be given about a positive or negative detection.

5.9.1 Phenolic compounds and aliphatic alcohols

Extraction and Cleanup. Analytical procedures employed for the extraction and cleanup of phenolic aromatic brominated compounds in biota like plasma and tissue samples can be based on methods developed for current-use BFRs. Several methods are described in the literature and can be easily adapted (for example Verrault, 2007). In general they base on separating an aqueous phase containing the deprotonated phenolics. The aqueous phase needs to be acidified to enable extraction of protonated phenolics and alcohols with an apolar organic solvent.

Table 11. Phenols and aliphatic alcohols

Substance Name	CAS No
1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester	20566-35-2
Tribromoneopentyl alcohol	1522-92-5
Dibromoneopentyl glycol	3296-90-0
2,4,6-tribromophenol	118-79-6

Subsequently, the phenolics need to be derivatized to their methoxylated (MeO) analogues, followed by a final cleanup prior analysis by GC/MS.

Other samples types might require different extraction methods, like accelerated solvent extraction (ASE), soxhlet and ultrasonic extraction with various solvent types and system parameters optimised for the best possible performance (e.g. extraction cycle s, time, and temperature).

However, adequate method adaptation relies on the availability of commercial reference standards. If standard compounds are not available only screening exercises are possible which base on the assumption that the analytical method for current-use BFR is applicable according to the similarity in chemical-physical properties and chemical structure. However, eventual losses during the analytical procedure cannot be uncovered and the compound of interest might not detectable without a prior validation of the method for new BFRs.

Analysis and Quantification. Derivatised phenolic brominated aromatic compound analyses and quantification can be performed using a gas chromatograph-mass spectrometer (GC-MS) operating in the electron capture negative ionization (ECNI) mode. The GC-MS(ECNI) analyte determination can be accomplished in the selected ion-monitoring (SIM) mode for the isotopic bromine anions 79Br- and 81Br-. Alternatively, a GC-highresolution MS in the electron ionization (EI) mode (GC-HRMS(EI)) can be applied. The GC-HRMS(EI) uses a MS system with a double focusing-magnetic sector mass analyzer operating at a mass resolution of 10 000 or greater with helium as a carrier gas.

If volatilisation in GC cannot achieved without breakdown of the compounds of interest, application of liquid chromatography combined with ultraviolet detection or MS methods can be used as well. Dibromoneopentyl glycol (DBNPG) concentration can be determined by high performance liquid chromatography (HPLC) with a ultraviolet diode array detector (DAD) G1315B and Lichrocart_250-4 HPLC-Cartrige Lichrosphere_ 100 rp-18 column. HPLC samples can be prepared by mixing DBNPG samples with HPLC-grade methanol (1:1). After centrifugation, the samples need to be filtered through a 0.45 lm membrane filter prior analysis. Tribromoneopentyl alcohol can maybe be analysed in a similar matter, however method optimisation would be needed.

However, due to the probable lack of commercially available standard compounds quantification of new BFRs can only be carried out by applying response factors of structurally similar chemicals. That will lead to semi-quantitative results biased by an elevated uncertainty. If no chemical with similar chemical structure is available either, only qualitative information can be given about a positive or negative detection.

5.9.2 Other organic brominated compounds

No analytical method could be found for tris(tribromoneopentyl) phosphate (CAS 19186-97-1), but a similar but modified method as used for tris(1,3-dichloro-2-propyl)phosphate (TDCP) could be applied. The inorganic compound ammonium bromide is a salt and is readily solved in water but could be analysed using ion exchange chromatography in a combination with detecting the bromide ions.

5.10 Screening strategies

Reports on the environmental screening of these "new" BFRs are scarce. Assuming that several new BFRs behave in a similar manner to known BFRs, future screening should be prioritized in similar "hot spots" and reference sites as for the well known prioritized BFRs, like penta-, octa- and deca-BDEs, TBBP-A and HBCDD. Examples of this are; electronic dismantling plants, areas where the industry have current use of these type of BFRs, landfills, waste water treatment plants, domestic and working environments.

To evaluate the environmental contamination potential of these selected BFRs a broad screening is suggested by studying:

- Emmisions to water - sewage treatment plants and run-off from landfills.

- Emmisions from point sources – marine and fresh water sediments from potential source areas as Drammenselva estuary (car demolition plants) and Ålesund area (upholstered furniture industry) and dust samples from electronic dismantling plants.

- Emissions to air - pine needles, bark, moss samples and passive air samples taken close to major urban areas.

- Exposure to humans - dust samples from the domestic and working environments should be sampled in order to detect the direct exposure to humans.

For more information on screening and sampling on these types of locations see SFT report 2367/2008 which describes the monitoring of phosphorous flame retardants, polyfluorinated organic compounds, nitro-PAHs, silver, platinum , and sucralose in air, waste treatment facilities, seawater, marine and fresh sediments, blue mussel and cod liver.

6. Prioritizing of compounds for further environmental monitoring

We have proposed a list of compounds potentially relevant for further monitoring by carefully evaluating current knowledge on these, from SFT, proposed BFRs. Priorities have been set based on the following criteria:

- Production volume (HPV or LPV)
- Product usage (additive, reactive intermediate or polymer)
- Long range transport potential (LRT potential)
- Bioaccumulation potential (BAP)
- Persistence
- Environmental levels
- Environmental transport processes

The prioritisation of chemicals has also involved sale volumes and sources for environmental release such as types of flame retarded products and other areas of use. Also, weight has been put on recent findings of these compounds in the environment such as the finding of "new" BFRs in aquatic animals.

Based on these criteria Appendix I was constructed to bring out the basic information needed to create such a prioritation list. The basis of the prioritization considered bioaccumulation as an important factor when available. Even if many of these BFRs are too heavy to be efficiently bioconcentrated they still can be found in the aquatic environment as is the case for BDE-209, as they usually are quite persistent in the environment. Also, while the studies involving the bioaccumulation and biomaginfication in the food web of these "new" BFRs are scarce, limited conclusions can be made on the few bioconcentration studies made. The selection relied more on the type of BFR (additive, reactive intermediates, polymer or unknown use) and production volume. The potential of this compound for long range transport is important but also if these BFRs are present in domestic environments and workplaces. Persistence albeit the persistence is mostly based on predictions, and is of limited value, when reactivity properties of compounds in eg. the atmosphere, is generally unknown. More importantly was our selection based on if any studies in the peer reviewed litterature have found these selected BFRs in the environment.

12 of the 21 "new" BFRs that were under investigation was listed, see Table 12, as potentially relevant for further investigation and monitoring in the Norwegian environment. In addition, 2,3-dibromopropyl-2,4,6-tribromophenyl ether (BPTE, CAS 35109-60-5) and 2-ethylhexyl-2,3,4,5-tetrabromobenzoate (TBB, CAS 183658-27-7) was added to the list. BPTE was selected as it is the main component of bromkal 73-5PE, and a propable reductive precursor of the priority compound; 2,4,6-Tribromophenyl allyl ether (ATE, CAS 3278-89-5). In addition, BPTE was one of the more prominent compounds in seal from the Barents Sea (see Chapter 1.1.1.1). TBB was selected as this is one of the major compounds in Firemaster 550 together with the priority compound Bis(2-ethylhexyl)tetrabromophtalate ((TBPH, CAS 26040-51-7)(see chapter 4.1.5.3).

Table 12. List of substances potentially relevant for further investigation and monitoring in the Norwegian environment. Two additional compounds (marked) not originally one of these 12 selected BFRs proposed as priority compound.

Compound name	***CAS no.***
Tetrabromobisphenol A bis(2,3-dibromopropyl ether)	21850-44-2

Tetrabromobisphenol A diallyl ether	25327-89-3
Hexabromobenzene (HBB)	87-82-1
Pentabromotoluene (PBT)	87-83-2
Pentabromoethylbenzene (PBEB)	85-22-3
2,4,6-Tribromophenyl allyl ether (ATE)	3278-89-5
2,3-dibromopropyl-2,4,6-tribromophenyl ether (DPTE)	35109-60-5
2,4,6-Tribromophenol (TBP)	118-79-6
Decabromodiphenylethane (DBDPE)	84852-53-9
1,2-Bis(2,4,6-tribromophenoxy)ethane (BTBPE)	37853-59-1
Ethylene bis(tetrabromophtalimide) (BTBPI)	32588-76-4
Tetrabromophtalic anhydride	632-79-1
Bis(2-ethylhexyl)tetrabromophtalate (TBPH)	26040-51-7
2-ethylhexyl-2,3,4,5-tetrabromobenzoate (PBB)	183658-27-7

The basis of the selection of the Tetrabromobisphenol A derivatives (CAS 21850-44-2 and
25327-89-3) is the type of usage of these BFRs, both being additive flame retardants (see chapter 4.1.1). They are classified as LPV compounds with a low potential for long range transport. Also, they probably have a low bioaccumulation potential as is generally the case with compounds having a molecular weight close to or more than 700 Dalton. Their persistent is probably high, especially as they will primarily be associated to particles in air, soil, dust, sediments and sludge, but as decaBDE might have the same transport mechanisms in the environment and thus as decaBDE become a global pollutant. In addition, as these compounds can be part of flame retarded products used in domestic and working environments, and little is known of their potential health impact. Unfortunately only a few peer reviewed publications is available (see chapter 4.1.1.1 and 4.1.1.2).

Similarly, the polyaromatic BFRs, Decabromodiphenylethane (CAS 84852-53-9) and 1,2-bis(2,4,6-tribromophenoxy)ethane (CAS 37853-59-1), is of interest based on the above mentioned reasons. Further, these compounds have been detected in the food web, air and tree bark around the Great Lakes (U.S.), in house dust, soil and sludge samples and in the arctic biota (see chapter 4.1.3.1 and 4.1.3.2).

Other compounds which might be categorized similary are 1,4-bis(pentabromophenoxy) tetrabromobenzene (CAS 58965-66-5), 2,4,6-tris(2,4,6-tribromophenoxy)-1,3,5-triazine (CAS 25713-60-4) and Tris(tribromoneopentyl)phosphate (CAS 19186-97-1) (see Table 13).

These compounds was not selected as priority compounds due to their size (>> 700 Da), as these compounds probably will have a low bioaccumulation potential and are difficult to analyse using standard methods for BFRs. In addition, 1,4-bis(pentabromophenoxy) tetrabromobenzene is used as a reactive intermediate and is a LPV compound (see chapter 4.1.3.3) while 2,4,6-tris(2,4,6-tribromophenoxy)-1,3,5-triazine lack any viable information on the type of usage (additive or reactive intermediate) or estimated volumes to make any clear conclusions (see chapter 4.1.3.4). Tris(tribromoneopentyl)phosphate is an additive but the lack of any information makes it hard to select this compound as a priority substance (see chapter 4.2.2.1). Further, there is no information in the peer reviewed literature on any of these three compounds or their environmental levels.

Both 1,4-bis(pentabromophenoxy)tetrabromobenzene and 2,4,6-tris(2,4,6-tribromophenoxy)-1,3,5-triazine might

degrade into more environmentally available compounds such as hexabromobenzene, pentabromophenol and 2,4,6-tribromophenol which might increase the amount of such antropogenic sources.

Ethylene bis(tetrabromophtalimide) (BTBPI, CAS 32588-76-4) was selected as a priority substance based on its usage as an additive, it is an HPV and is not readily biodegradable (see chapter 4.1.5.1 and Table 12) and might be persistent in the environment. The potential for long range transport, bioaccumulation and bioconcentration would propably be low due to its size (Mw >> 700).

Table 13. List of compounds not included in the priority list.

Compound name	***CAS no.***
Dibromostyrene	125904-11-2
Pentabromobenzyl acrylate	59447-55-1
1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl	20566-35-2
Tribromoneopentyl alcohol	1522-92-5
Dibromoneopentyl glycol	3296-90-0
Tris(tribromoneophentyl)phosphate	19186-97-1
Ammoniumbromide	12124-97-9

Hexabromobenzene (CAS 87-82-1), pentabromotoluene (CAS 87-83-2), pentabromoethylbenzene (CAS 85-22-3) and 2,4,6-tribromophenol (CAS 118-79-6) is included in the list in table 12, as they all have a high potential for long range transport. They are bioavailable for bioconcentration and bioaccumulation even if some show a high degree of metabolism in animal studies (see chapter 4.1.2) and will propably have a low persistence in the atmosphere. Generally, they have been detected in the foodweb and arctic regions.

The polymers (see Ch. 4.1.4) were not considered as priority substances since their persistence propably are low. Further, they are quite volatile and might therefore degrade in the atmosphere. There is also a lack of information on their occurrence in the environment.

The alcohols (see Ch. 4.2.1 and Table 13) were not considered as they are reactive intermediates and LPV. They are mainly distributed in the environment in the aqueous phase. Further, their persistence was predicted to be low as well as the bioaccumulation potential due to the low log K_{ow}. In addition no information is available in the peer reviewed literature on the environmental concentrations.

Tetrabromophtalic anhydride (CAS 632-79-1) and bis(2-ethylhexyl)tetrabromophtalate (TBPH, CAS 26040-51-7) are both additive BFRs and LPV chemicals. Predictions (see chapter 5) suggest a low propability for long range transport for any of the chemicals while tetrabromophtalic anhydride have in studies show an medium to average BCF, see chapter 1.1.1.1, while their persistency is unknown the predictions suggest an half-life of 372 and 173 days, respectively. Tetrabromophtalic anhydride was suggested to have an arctic contamination potential while there is no studies that have, to our knowledge, found this compound in environmental samples. TBPH on the other hand have been detected in dust and sludge (see chapter 4.1.5.3) and also 2-ethylhexyl-2,3,4,5-tetrabromobenzoate (TBB) which is also a component of Firemaster 550 and should be considered for inclusion in a screening process.

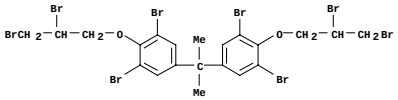
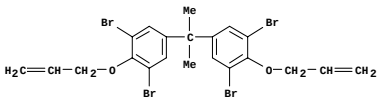
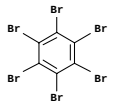
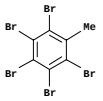
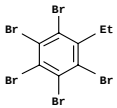
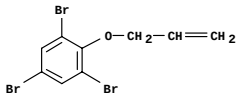
7. Units and abbreviations

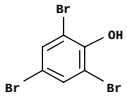
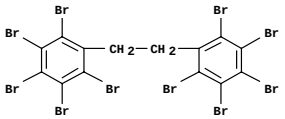
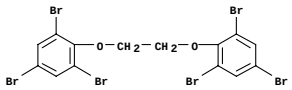
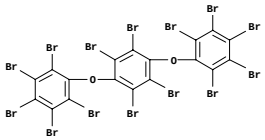
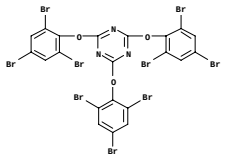
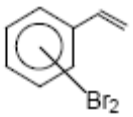
°C	degrees Celsius
µg	microgram(s)
µg/ml	microgram(s) per milliliter
Φ_{Air}	estimated particle bound-fraction in the atmosphere
ABS	Acrylonitrile butadiene styrene terpolymer
AC-BAP	arctic contamination and bioaccumulation potential
AhR	arylhydrocarbon receptor or dioxin receptor
BCF	bioconcentration factor
BFR	Brominated Flame Retardant
BMF	biomagnification factor
BOD	biochemical oxygen demand
CAS	chemical abstracts service
CTD	characteristic travel distance
Da	Dalton (1 Dalton = 1 unit of mass)
$eACP_{10}^{air}$	Arctic contamination potential for a substance after 10 years of continuous emissions to the atmosphere
EPA	Environmental Protection Agency
FR	Flame Retardant
g	gram(s)
g/kg	gram(s) per kilogram
g/l	gram(s) per litre
g/ml	gram(s) per milliliter
g/mol	gram(s) per mole
GC/MS	gas chromatography/mass spectrometry
HIPS	high-impact polystyrene
HPV	high production volume
i.v.	intravenous
l	liter(s)
LC_{50}	concentration lethal to 50% of test animals
LD_{50}	dose lethal to 50% of test animals
log K_{AW}	logarithm of the air-water partitioning coefficient
log K_{OA}	logarithm of the octanol-air partitioning coefficient
log K_{OC}	logarith of the octanol-carbon partitioning coefficient
log P_{OW}	logarithm of the octanol-water partitioning coefficient
LOQ	limit of quantification
LPV	low production volume
LRT	long range transport
LRTP	long range transport potential
m^3	cubic metre
MLOQ	method limit of quantification
mg	milligram(s)
mg/kg	milligram(s) per kilogram(s)
ng/g	nanogram(s) per gram(s)
ND	not detected
NIOSH	National Institute for Occupational Safety and Health
NOEL	No Observed Effect Level
NOAEL	No Observed Adverse Effect Level

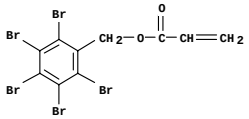
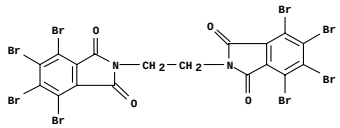
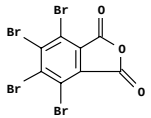
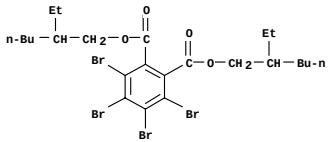
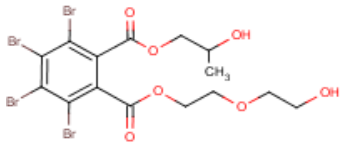
OECD	Organisation for Economic Co-operation and Development
Pa	vapour pressure in Pascal
PBT	Polybutyleneterephatlate
PET	Polyethylene terephatale
pg/m^3	picogram(s) per cubic metre
pK_a	acid dissociation constant
Pov	overall persistence
ppb	part per billion
ppm	part per million
TCLo	Lowest published lethal concentration
TDLo	Lowest published lethal dose
TE	transfer efficiency
wt	weight
WWTP	waste water treatment plants

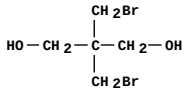
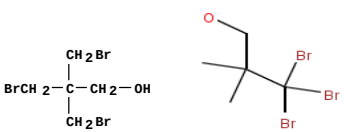
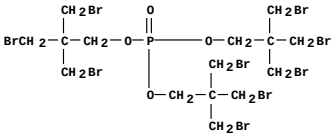
8. Appendix I

Summary of compound specific information and estimated environmental properties.

Names	CAS no.	Structure	Type of BFR[a]	Estimated volumes[b]	Analysis[c]	LRT potential[d]	BioAcc Potential[e]	Environmental transport processes[f]			Persistence[g]	Literature[f]
Aromatics								**Air**	**Water**	**Particles**		
Tetrabromobisphenol A derivatives												
Tetrabromobisphenol A bis(2,3-dibromopropyl ether)	21850-44-2		Additive	LPV	[1]	Low	Low Mw>700			Single hopper	P_{OV} >500 days	Dust
Tetrabromobisphenol A diallyl ether	25327-89-3		Additive Reactive	LPV	[1]	Low	Low Mw=624			Single hopper	P_{OV} >500 days Resistant to oxidation	No data
Benzenes/Phenols												
Hexabromobenzene	87-82-1		N/A	N/A	[1]	High	High BCF < 1	Multi hopper/ Single hopper			P_{OV} >500 days Degrading in atm UV	Global pollutant Arctic
Pentabromotoluene	87-83-2		N/A	LPV	[1]	High	High BCF < 39	Multi-hopper/ Single hopper			P_{OV} >500 days Degrading in atm UV?	Arctic
Pentabromoethylbenzene	85-22-3		Additive	LPV	[1]	High	High BCF < 1	Multi-hopper/ Single hopper			P_{OV} >500 days Degrading in atm UV?	Arctic
2,4,6-Tribromophenyl allyl ether	3278-89-5		Reactive	LPV	[1]	High	Low	Multi-hopper			P_{OV} 168 days Atm $t_{1/2}$ <1day	Seal Sludge

Names	CAS no.	Structure	Type of BFR[a]	Estimated volumes[b]	Analy-sis[c]	LRT poten-tial[d]	BioAcc Potential[e]	Environmental transport processes[f]			Persist-ence[g]	Litte-rature[f]
2,4,6-tribromophenol	118-79-6		Reactive inter-mediates	HPV	[2]	High *Low for deproto-nated pK_a 6.34*	High BCF =204 *Low for deproto-nated*	Multi-hopper	*Deproto-nated Swimmer*		Anaerobic degrada-tion Atm $t_{1/2}$ = 34 days	Fish Soil WTTP
Polyaromatics												
1,2-bis(pentabromo-phenyl) ethane	84852-53-9		Additive	N/A	[1]	Low	Low Mw>700 BCF<2.5			Single-hopper	P_{OV} >500 days	Fish Bird eggs Dust WWTP
1,2-bis(2,4,6-tribromo-phenoxy)ethane	37853-59-1		Additive	LPV	[1]	Low	Mw≈700 HighBMF Low up-take and metab			Single-hopper	P_{OV} >500 days	Mus-sels Fish Dust Arctic
1,4-bis(pentabromophenoxy) tetrabromobenzene	58965-66-5		Reactive inter-mediate	LPV	[1?]	Low	Low Mw>>700			Single-hopper	P_{OV} >500 days	No data
2,4,6-Tris(2,4,6-tribromo-phenoxy)-1,3,5-triazine	25713-60-4		N/A	N/A	[1]	Low	Low Mw>>700			Single-hopper	P_{OV} >500 days	No data
Polymers												
Benzene, ethenyl-, aryl bromo derivatives (Dibromostyrene, 85%)	125904-11-2 31780-26-4		Polymer	N/A	[1]	High	Atm $t_{1/2}$ <1day	Multi hopper	Swimmer		P_{OV} = 95 days Hy-dro-lysis = 59 days	No data

Names	CAS no.	Structure	Type of BFR[a]	Estimated volumes[b]	Analysis[c]	LRT potential[d]	BioAcc Potential[e]	Environmental transport processes[f]			Persistence[g]	Literature[f]
Pentabromobenzyl acrylate (as monomer) Poly(pentabromobenzyl)-acrylate (as polymer)	59447-55-1		Reactive intermediate Polymer	LPV	[1]	Borderline	High	*Multi hopper*		*Single hopper*	P_{OV} >500 days? Atm $t_{1/2}$ <1day	No data
Others												
Ethylene bis tetrabromophtalimide	32588-76-4		Additive	HPV	[1]	Low	Low Mw>700 Low BCF			Single hopper	P_{OV} >500 days Not biodegradable	No data
Tetrabromophtalic anhydride	632-79-1		Additive, reactive intermediates for polyols, esters and imides	LPV	[1]	Low	BCF=439	Multi hopper		Single hopper	P_{OV} = 372 days	No data Suggested to be an arctic contam.
Bis(2-ethylhexyl)tetrabromophtalate	26040-51-7		Additive	LPV	[1]	Low	Low Mw≈700			Single hopper	P_{OV} = 173 days	Dust WWTP
Alifatics												
Alcohols												
1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl ester	20566-35-2		N/A	N/A	[2]	Low	Low Mw=628			Single hopper	P_{OV} = 172 days	No data

Names	CAS no.	Structure	Type of BFR[a]	Estimated volumes[b]	Analysis[c]	LRT potential[d]	BioAcc Potential[e]	Environmental transport processes[f]			Persistence[g]	Literature[f]
Dibromoneopentyl glycol	3296-90-0		Reactive intermediates	LPV	[2]	Low	Low $logK_{ow}$= 0.39		Swimmer		P_{OV} = 31 days	No data
1-Propanol, 2,2-dimethyl-, tribromo derivative or Tribromoneopentyl alcohol	36483-57-5 1522-92-5		Reactive intermediates	N/A	[2]	Low	Unknown log Kow =2.5		Swimmer		P_{OV} = 91 days	No data
Phosphorous flame retardant												
Tris(tribromoneopentyl) phosphate	19186-97-1		Additive	N/A	[1]	Low	Low Mw>700			Single hopper	P_{OV} >500 days	No data
Inorganic												
Ammoniumbromide	12124-97-9	NH4Br	Filler	HPV		N/A	N/A	N/A	N/A	N/A	N/A	No data

a) Flame retardants are either used as additives, reactive intermediates or polymers in flame retarded materials; **b)** Estimated production volumes; HPV=high production volume, LPV=low production volume; **c)** Method of sample preparation and analysis; [1]= neutral method as defined in chapter 6.3; [2] = phenolic method as defined in chapter 6.3.1; **d)** Long range transport (LRT) potential as defined in chapter 5; **e)** The potential for BFRs to bioconcentrate/accumulate. Information based on literature data and the assumption that the bioconcentration/accumulation siginficantly decreases for molecules with molecular weights over 700 Dalton; **f)** Environmental transport processes of chemicals defined as single and multiple hoppers and swimmers see chapter 5.3; **g)** Persistence defined as the overall persistence (P_{OV}) from calculated degradation rates in air, water and soil done in EPISuite, see Table 7; **h)** Information extracted from the literature where these BFRs have been detected, eg. in dust from homes or workplaces, waste water treatment plants (WWTP), fish from rivers, lakes or the sea, BFRs detected in arctic samples such as gulls from the Norwegian arctic or seals from the Barets sea.

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Utførende institusjon Norsk institutt for luftforskning (NILU)	Kontaktperson SFT Stine Husa	ISBN-nummer 978-82-425-2091-3 (T) 978-82-425-2092-0 (E)

	Avdeling i SFT Kjemikalieavdelingen	TA-nummer 2462/2008

Oppdragstakers prosjektansvarlig Mikael Harju (NILU)	År 2008	Sidetall 120	SFTs kontraktnummer 3008054

Utgiver Norske institutt for luftforskning (NILU) NILU OR 16/2009	Prosjektet er finansiert av Statens forurensingstilsyn (SFT)

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Tittel - norsk og engelsk

Current State of Knowledge and Monitoring requirements for emerging ”new” brominated flame retardants in flame retarded products and the Environment

Miljømessig kunnskapsstatus og overvåkingsbehov for ”nye” bromerte flammehemmere i flammehemmede materialer og i miljøet

Sammendrag – summary

This report summarises the current state of knowledge on types, market volumes, manufacturers, suppliers and uses of brominated flame retardants of selected “new” BFRs. The accumulated knowledge of their physicochemical properties, potential health and environmental effects is also summarised. Further the potential of these “new” BFRs to become Arctic contaminants is assessed using partitioning properties and figures relating these partitioning properties to maps defining modes of transport and arctic contamination and bioaccumulation potential. The assessment also takes into account estimates of the persistence of these BFRs in the different environmental compartments.

The report concludes with a summary of the current sampling and analysis techniques and finally the prioritisation report, suggesting which BFRs should be selected as priority compounds for an environmental screening.

4 emneord BFH, langtransportpotential, prioritetsliste, analyser	4 subject words BFR, long range transport potential, priority list, analysis

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TA-2462/2008
ISBN: 978-82-425-2091-3 (T)
ISBN: 978-82-425-2092-0 (E)