



**TSCA Work Plan Chemical
Technical Supplement – Physicochemical Properties and
Environmental Fate of the Brominated Phthalates Cluster
(BPC) Chemicals**

**Brominated Phthalates Cluster
Flame Retardants**

CASRN	NAME
26040-51-7	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1,2-bis(2-ethylhexyl) ester
183658-27-7	Benzoic acid, 2,3,4,5-tetrabromo-, 2-ethylhexyl ester
20566-35-2	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1-[2-(2-hydroxyethoxy)ethyl] 2-(2-hydroxypropyl) ester
77098-07-8	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol
7415-86-3	1,2-Benzenedicarboxylic acid, 1,2-bis(2,3-dibromopropyl) ester
*	Confidential A
*	Confidential B

* Confidential Business Information

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1 INTRODUCTION

Each chemical in this cluster has several structural features in common:

- 1) Multiple bromine atoms, typically attached to the aromatic ring
- 2) The 1,2-benzenedicarboxylate moiety (phthalate structure)¹ and
- 3) Alkyl esters

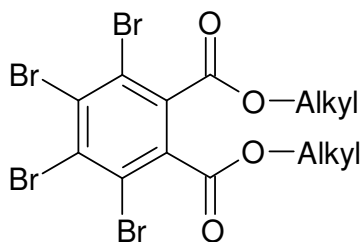


Figure 1-1: Generic Structure of the Brominated Phthalates Cluster Chemicals

Some members of the cluster have free primary or secondary alcohol functionalities. These may impart certain properties to the chemical substance [making them more water soluble and chemically reactive], more significantly the alcohol moiety can react to incorporate the brominated (BFR) into the substrate via covalent bond formation. These chemicals are not limited to that reactive form of application and they could also be mixed with substrate as an additive flame retardant (FR).

The one cluster member is an anomaly when compared to the structure of the other cluster member chemicals, *bis* (2,3-dibromopropyl) 1,2-benzenedicarboxylic acid (CASRN 7415-86-3). The primary difference between this chemical and the other cluster members is the positioning of the four (4) bromine atoms (on the alkyl ester moieties) as opposed to the positions on the benzene ring.

¹ The cluster member 2-ethylhexyl-2,3,4,5-tetrabromobenzoate (**TBB**; CASRN 183658-27-7) is missing one of the phthalate carboxylate ester but is including in this cluster since the commercial product Firemaster 550 also contains the **TBB** / **TBPH** phthalate mixture. This structural anomaly should not affect the inclusion of this chemical since phthalates often decarboxylate during metabolism and biodegradation. (Robbert Kleerebezem*, 1999)

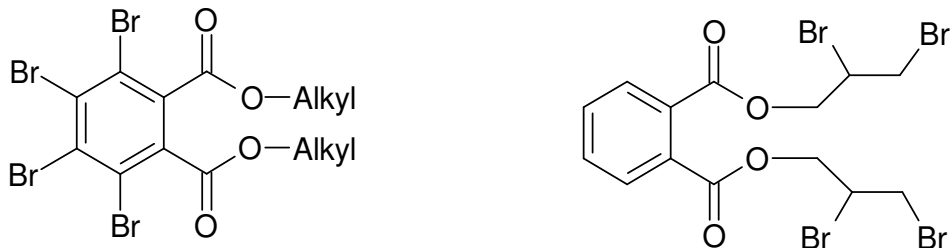


Figure 1-2: Generic structure of the BPC members and CASRN 7415-86-3

1.1 CHEMICAL AND PHYSICAL PROPERTIES

1.1.1 Reactive BPC members

The reactive members of the BPC are 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1-[2-(2-hydroxyethoxy)ethyl] 2-(2-hydroxypropyl) ester (**TBPA-Diol**; CASRN 20566-35-2) and 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol (**TBPA-Diol**; CASRN 77098-07-8).

Because these chemicals are chemically bound to the polymer, it is far less likely they will migrate from products or articles unless there is excess chemical present due to an incomplete polymerization reaction. The reactive members of the brominated phthalates cluster (BPC), including the primary degradation product tetrabromophthalic acid, have not been reported in literature as being present in environmental or biological media.

The brominated phthalates with hydroxyalkyl esters are generally intended to react with isocyanate monomers and become covalently bonded into the chemical backbone of the polyurethane foams (PUF). There is no evidence of the phthalate esters based urethane linkages ever depolymerizing under abiotic, biotic, or metabolic conditions. One may anticipate that if depolymerization were to occur the ester linkage would cleave before the carbamate linkage generating the tetrabromophthalate diacid as a predominant product. There has been no monitoring data indicating the presence of hydroxyalkyl tetrabromophthalates in the environment or biota. As such worker exposures would be the main concern during chemical manufacturing and PUF manufacturing. The esters are liquids with negligible vapor pressure and limited but measurable water solubility because of the hydroxyl and/or other oxygen atoms in the molecule [one MSDS states < 1 g/L; the estimates are substantially lower than this number but seem unreasonable]. In one patent [Crain and Surma, 2010], it is noted that both reactive and additive BPC chemicals can be added to foam, which would again lead to potential release of one type of BPC while the reactive BPC would be self contained in the foam backbone.

1.1.2 Additive BPC members

The additive members of the BPC are 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1,2-bis(2-ethylhexyl) ester (**TBPH**; CASRN 26040-51-7), benzoic acid, 2,3,4,5-tetrabromo-, 2-ethylhexyl ester (**TBB**; CASRN 183658-27-7) and 1,2-Benzenedicarboxylic acid, 1,2-bis(2,3-dibromopropyl) ester (CASRN 7415-86-3).

Additive flame retardants are incorporated and dispersed throughout a product, but are not chemically bound to it. Additive flame retardants are more likely than reactive flame retardants to migrate from products or articles. Emissions from a single product or article may be small. However, combined emissions from all sources within various indoor microenvironments, residences, schools, public and commercial buildings, cars, trains, airplanes, may be significant.

TBPH and **TBB** are liquids with negligible vapor pressure and water solubility. They have the same functional groups and may be considered close analogs of one another.

There are few measured physicochemical properties values for Melting Point, Boiling Point, Vapor Pressure, Water Solubility or Octanol Water Partition Coefficient for these chemicals. The MSDS sheet (Unitex, 2006) for pure **TBPH** provides some range limits for the cluster as does the water solubility [1.3 mg/L at 25°C, (ECHA, 2013)] for the unbrominated di(2-ethylhexyl) phthalate (DEHP) ; while the more water soluble products [hydroxyl containing] are represented by **CASRN 77098-07-8**, a submission under the HPV Challenge program (Albemarle - GLCC, 2004).

Table 1-1: Physicochemical properties of TBPH

Compound	MP	BP	VP	s-H2O	Log Kow
TBPH	< -20 °C	> 400 °C	< 1.0 E-3 Torr at 25 °C	insoluble	9.34 (ACD est.)

Source: Unitex Chemical Corp. Uniplex FRP-45 MSDS (Unitex, 2006)

Table 1-2: Physicochemical Properties of TBPA Diol

Compound	MP	B	V	s-H2O	Log Kow
CASRN 77098-07-8	NA	N A	< 1E-6 Torr (est.)	< 1 g/L MS	3.83 (EPI est.)

Source: EPA HPV Challenge Program submission (Albemarle - GLCC, 2004)

CASRN 7415-86-3

No data were located for this cluster member.

In addition to the chemicals already described, **Confidential A**, and **Confidential B** can be considered analogous to the other cluster members described here. There was little to no physicochemical data, and structures for these chemicals are similar enough to use read across.

1.2 ENVIRONMENTAL FATE AND BIOACCUMULATION

1.2.1 Summary

Very little information exists on the environmental fate and bioaccumulation of the brominated phthalates cluster (BPC) members. 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1,2-bis(2-ethylhexyl) ester (**TBPH**) and benzoic acid, 2,3,4,5-tetrabromo-, 2-ethylhexyl ester (**TBB**) are the best studied and may be considered close analogs of one another. Based on available data, both compounds are ranked low for persistence (P1) relative to standard criteria (EPA, 1999b). The tetrabrominated microbial degradation and/or hydrolysis products tetrabromophthalic acid and tetrabromobenzoic acid are expected to be much more persistent and are ranked as P3. Estimated bioaccumulation factors (BAFs) suggest that **TBPH** and **TBB** have low (B1) and moderate bioaccumulation potential (B2), respectively. The phthalic and benzoic acid products are also considered to have low (B1) and moderate bioaccumulation potential (B2), respectively.

TBPH and **TBB** are expected to have low mobility in soil. Biodegradability is not well characterized but based on available data, half-lives for primary degradation in water may be on the order of days. Primary biodegradation of **TBPH** and **TBB** is expected to yield the monoethylhexyl ester of tetrabromophthalic acid and tetrabromobenzoic acid as the main products, respectively. Abiotic hydrolysis may occur, but the low solubility of **TBPH** and **TBB** may lower the effective rate of hydrolysis in the environment. Based on estimated half-lives and considering the low water solubility, rates of abiotic hydrolysis are expected to be negligible at environmental pH and temperatures. The ultimate hydrolysis products of **TBPH** and **TBB**, 3,4,5,6-tetrabromo- 1,2-benzenedicarboxylic acid (i.e. tetrabromophthalic acid) and tetrabromobenzoic acid, are expected to be resistant to further abiotic transformations as well as biodegradation and may be persistent in the environment. The rate of atmospheric gas-phase (hydroxyl radical) photo-oxidation has the potential to be moderate; however, these substances are expected to exist primarily in the particulate phase in the ambient atmosphere, and generally it is assumed that oxidation of particle-bound substances is slow or negligible. Particulate-phase **TBPH** and **TBB** are expected to be removed from the atmosphere by wet and dry deposition processes. **TBPH** and **TBB** absorb light at environmentally significant wavelengths, but the importance of this process for environmental waters has not been established. These chemicals have the potential to be transported far from their original point of release, primarily in the atmospheric particle-bound form.

1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1-[2-(2-hydroxyethoxy)ethyl] 2-(2-hydroxypropyl) ester and 1,2-benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with

diethylene glycol and propylene glycol (CASRN 77098-07-8 and 20566-35-2) are expected to have high mobility in soil. Estimated abiotic hydrolysis half-lives for this substance are lower than for **TBPH** and **TBB** (on the order of days to months depending on the estimation program), but these values are still considered to be in the slow-to-negligible category (EPA, 2012f). No biodegradation data were available for this substance. Given its molecular structure this substance would not be expected to be readily biodegradable, but both abiotic hydrolysis and biodegradation may produce the same brominated degradation product as for **TBPH**; namely tetrabromophthalic acid. As for **TBPH** and **TBB**, the estimated rate of atmospheric photooxidation is moderate; however, this is not expected to be an important environmental degradation pathway. Given the estimated rate of hydrolysis, CASRN 77098-07-8 is expected to have low persistence (P1) and low bioaccumulation potential (B1). However, the degradation product tetrabromophthalic acid is expected to have high persistence (P3) and low bioaccumulation potential (B1).

No measured environmental fate data exist for 1,2-benzenedicarboxylic acid, 1,2-bis(2,3-dibromopropyl) ester, CASRN 7415-86-3. Both estimated vapor pressure and volatility, based on estimated Henry's Law constant, are low. This substance is expected to partition strongly to environmental solid phases (in sludge, soil, etc.) and have low-to-moderate mobility in soil. Based on chemical structure and estimated data hydrolysis may occur, but the rate is expected to be negligible. Given its molecular structure this substance would not be expected to be readily biodegradable. Atmospheric photooxidation is expected to be slow. This substance is estimated to be moderately persistent (P2) and bioaccumulative (B2). Hydrolysis, if it occurs, may yield 2,3-dibromopropanol as a product, but neither this nor any other hydrolysis products are expected to have PBT properties.

1.2.2 Fate in Air and the Indoor Environment

BPC members have low-to-negligible vapor pressures and low-to-negligible volatility, and as a result, inhalation of volatilized (gas phase) substances is expected to be a minor route of indoor exposure for all BPC members. In contrast exposure via dust may be important, but little information is available on how these compounds get into house dust. This process may involve direct transfer from flame-retarded objects, driven by partitioning properties of the substances. Measured concentrations of **TBPH** (Ali et al., 2012; Allen et al., 2013a; Allen et al., 2013b; Bradman et al., 2012; Dodson et al., 2012; Gheorghe et al., 2013; Johnson et al., 2013; Kopp et al., 2012; Sahlstrom et al., 2012; Schlabach et al., 2011; Shoeib et al., 2012; Springer et al., 2012; Stapleton et al., 2008a; Stapleton et al., 2009; Stapleton et al., 2008b; Van den Eede et al., 2012) and **TBB** (Ali et al., 2012; Allen et al., 2013a; Allen et al., 2013b; Bradman et al., 2012; Dodson et al., 2012; Gheorghe et al., 2013; Johnson et al., 2013; Kopp et al., 2012; Sahlstrom et al., 2012; Schlabach et al., 2011; Shoeib et al., 2012; Springer et al., 2012; Stapleton et al., 2008a; Stapleton et al., 2009; Stapleton et al., 2008b; Van den Eede et al., 2012) in indoor air and dust are consistent with these predictions. The relative contributions of indoor air and dust to overall exposure indoors are expected to be similar to that reported for polybrominated diphenyl ethers (PBDEs) in the indoor environment (Webster et al. 2013), for which dust was considered important but indoor air not.

If released to the ambient atmosphere, these compounds are expected to exist primarily in the particulate phase, given their estimated vapor pressures. Consequently, the photochemically catalyzed vapor phase reaction with hydroxyl radicals (for which half-lives are given in Table 1-3) is not expected to be environmentally relevant. Davis and Stapleton (2009) measured half-lives for photodegradation of **TBPH** and **TBB** by sunlight in several organic solvents. Half-lives for photodegradation of **TBPH** in toluene, methanol, and tetrahydrofuran were 147, 220 and 168 min, respectively. For **TBB** the values were 162, 95, and 85 min. These results suggest that both substances absorb light and photodegrade at environmentally important wavelengths, although for water the importance of this process is not known.

In the particulate phase, they may be subject to removal from the atmosphere via wet or dry deposition. **TBB** and **TBPH** have the potential to be transported far from their original point of release (Harju et al., 2009), but their atmospheric transport behavior is determined by the transport behavior of the particles to which they sorb. A study of arctic biota by Harju *et al.* (2009) provides supporting evidence of long-range transport. In an air monitoring study **TBPH** and **TBB** were detected at high frequency in samples collected from North America, Central and South America, Europe, Africa, Asia, and Australia (Lee et al., 2010), providing additional evidence for the ability of these substances to enter the atmosphere and undergo long-range transport.

CASRN 77098-07-8 and 20566-35-2, and CASRN 7415-86-3 are expected to behave similarly to **TBPH** and **TBB** in the atmosphere. The estimated Henry's Law constants are negligibly low (Table 1-3) and as a result, they are not expected to volatilize from water or soil. However, even if released to the atmosphere, they are expected to exist primarily in the particulate phase. Consequently, the photochemically catalyzed vapor phase reaction with hydroxyl radicals is not expected to be environmentally relevant.

1.2.3 Fate in Water

If released to water, **TBPH** and **TBB** are expected to adsorb to sediment and suspended particulate matter, based upon the estimated K_{oc} values (Table 1-3). Volatilization from water is not expected to be an important environmental fate process given the estimated Henry's Law constants. Abiotic hydrolysis may occur, but the low solubility of **TBPH** and **TBB** may lower the effective rate of hydrolysis in the environment. Based on estimated half-lives and considering the low water solubility, rates of abiotic hydrolysis are expected to be negligible at environmental pH and temperature. The ultimate hydrolysis products of **TBPH** and **TBB**, 3,4,5,6-tetrabromo-1,2-benzenedicarboxylic acid (i.e. tetrabromophthalic acid) and tetrabromobenzoic acid, respectively, are expected to be resistant to further abiotic transformation as well as biodegradation and may be persistent in the environment.

TBPH was not readily biodegradable in one test, achieving less than 4% of its theoretical oxygen demand after 28 days in a test with inoculum from secondary effluent from a tricking filter at a sewage treatment plant that received predominantly domestic waste (Table 1-3). It is unclear

whether these results represent a combination of a closed bottle test (OECD TG 301D) and a modified Sturm test (OECD TG 301B), or two separate tests. In a separate Porous Pot test (OECD TG 303A) conducted using a commercial mixture of **TBPH** and **TBB**, these substances did not biodegrade but did show substantial total removal ($\geq 93\%$) by sorption to sludge.

Primary biodegradation of **TBPH** and **TBB** is expected to yield the monoethylhexyl ester of tetrabromophthalic acid and tetrabromobenzoic acid as the main products, respectively. A shake-flask die-away study (OCSP 835.3170) of the same commercial mixture yielded half-lives for disappearance of the starting material of 3.5 days and 8.5 days in active water and active sediment test systems, respectively. Neither ultimate degradation nor other possible metabolites were measured in this test.

Recently de Jourdan *et al.* (de Jourdan *et al.*, 2013) studied the fate of **TBPH** and **TBB** in aquatic mesocosms, which are designed to closely simulate environmental conditions. This type of study can be considered a higher tier (more realistic) form of simulation test, in comparison to die-away studies as summarized above. The median dissipation times (DT50) differed in the two compartments, with more rapid disappearance in the particulate (9–30 d) than in the sediment compartment (>100 d) for each compound. The degradation products were more concentrated in the particulate compartment and corresponded to known photodegradation products. The ratio of **TBB** to **TBPH** differed in the mesocosm compartments compared with the starting test material, indicating increased degradation of **TBB** relative to **TBPH**. In the die-away test (discussed in the preceding paragraph) the “active sediment” treatment had a low level of suspended sediment in natural water; thus it is analogous to the “particulate phase” treatment in the de Jourdan *et al.* (de Jourdan *et al.*, 2013) mesocosm study. The reported DT50s of 9–30 d for the particulate compartment therefore can be compared to the 8.5-day half-life for the “active sediment” die-away treatment. The higher DT50s observed in the “sediment phase” portion of the mesocosm study would be expected, given that as a rule, organic chemicals degrade more slowly under the anaerobic conditions prevalent in benthic sediments.

Davis and Stapleton (Davis and Stapleton, 2009) measured half-lives for photodegradation of **TBPH** and **TBB** by sunlight in several organic solvents. Half-lives for photodegradation of **TBPH** in toluene, methanol, and tetrahydrofuran were 147, 220 and 168 min, respectively. For **TBB** the values were 162, 95, and 85 min. These results suggest that both substances absorb light and photodegrade at environmentally important wavelengths, but the importance of this process for the water environment is not known. The observation by de Jourdan *et al.* (2013) that mesocosm degradation products corresponded to known photodegradation products is consistent with Davis and Stapleton (Davis and Stapleton, 2009), but again, photodegradation has not been directly studied under environmentally relevant conditions.

Estimated abiotic hydrolysis half-lives for 3,4,5,6-tetrabromo-1,2-benzenedicarboxylic acid, mixed esters with diethylene glycol and propylene glycol (CASRNs 77098-07-8 and 20566-35-2) are lower than for **TBPH** and **TBB** (on the order of days to months depending on the estimation program), but still considered to be in the slow-to-negligible category. No biodegradation data

were available for this substance. Given its molecular structure it would not be expected to be readily biodegradable, but both abiotic hydrolysis and biodegradation may produce the same brominated degradation product as for **TBPH**; namely tetrabromophthalic acid. The nonbrominated ester hydrolysis product(s) of 3,4,5,6-tetrabromo-1,2-benzenedicarboxylic acid, mixed esters with diethylene glycol and propylene glycol are expected to be rapidly biodegradable under all conditions. 1,2-(2,3-Dibromopropyl) benzene dicarboxylate (CASRN 7415-86-3) is estimated to hydrolyze abiotically more slowly than other cluster members (i.e. at a negligible rate) but is similarly not expected to be readily biodegradable. Abiotic or biologically catalyzed hydrolysis, if either occurs, may yield 2,3-dibromopropanol as a product.

1.2.4 Fate in Soil and Sediment

If released to soil, **TBPH** and **TBB** are expected to have low mobility, based on their estimated log K_{oc} values. Estimated K_{oc} values for 1,2-(2,3-dibromopropyl) benzene dicarboxylate (CASRN 7415-86-3) are just below the threshold for low/moderate mobility, suggesting that mobility may be characterized as low-to-moderate for this cluster member. In contrast, 3,4,5,6-tetrabromo-1,2-benzenedicarboxylic acid, mixed esters with diethylene glycol and propylene glycol (CASRN 77098-07-8 and 20566-35-2) is expected to have high mobility in soil. The biodegradation studies and other evidence discussed above suggest that ultimate degradation of the brominated benzoic and phthalic acid degradation products of BPC members is likely to be slow. One study is available for tetrabromophthalic anhydride (CASRN 632-79-1), which would be quickly hydrolyzed to tetrabromophthalic acid (CASRN 13810-83-8) in the environment, and it showed no degradation in 28 days (Butz, 1979). The nonbrominated products that would be formed from biological or abiotic hydrolysis of the parent materials are expected to biodegrade easily under all environmental conditions. Volatilization from moist soil surfaces is expected to be low given the negligibly low estimated Henry's Law constants (Table 1-3). Hydrolysis may be an important environmental fate process in moist soil but this requires experimental confirmation.

Davis (Davis, 2013) studied the fate of **TBPH** and **TBB** in greenhouse experiments. These compounds were found to resist degradation biosolids-amended, in non-vegetated soil, but in biosolids-amended soil planted with alfalfa, 43% of **TBPH** was lost in 28 days in the high biosolids-amended pots. It was stated that no clear evidence of phytoaccumulation was observed, suggesting that **TBPH** loss was due to degradation in the soil.

1.2.5 Bioaccumulation

A commercial mixture of **TBPH** and **TBB** served as the test substance in a rainbow trout bioconcentration study. The whole-fish measured bioconcentration factor (BCF) for the mixture was 2.02 (log BCF = 0.31). Steady state was achieved in that study, which used uptake and depuration periods of 35 and 14 d, respectively. Estimated BAFs (BCFBFAF v3.00) suggest low bioaccumulation potential (B1) for **TBPH** but moderate potential (B2) for **TBB** (Table 1-3). BCFBAF calculates a metabolic transformation half-life normalized to a 10g fish and the ester linkage has the largest negative fragment coefficient, suggesting this may be the primary site of

transformation for **TBPH** and **TBB**. However, metabolic biotransformation via debromination in fish could also reduce bioaccumulation (Stapleton et al., 2004). (Sagerup et al., 2010) observed apparent trophic magnification of **TBB**, but not **TBPH**, in an Arctic food chain in Svalbard, Norway. The food chain included one fish species, capelin (*Mallotus villosus*); three seabird species: common eider (*Somateria mollissima*), Brünnich's guillemot (*Uria lomvia*), and black-legged kittiwake (*Rissa tridactyla*); and three mammalian species: ringed seal (*Phoca hispida*), Arctic fox (*Vulpes lagopus*), and polar bear (*Ursus maritimus*). **TBB** was detected in all seven species and **TBPH** in five of the seven species at ng/g levels. Lipid-adjusted concentrations did not scale with trophic level with the exception of TBB, which was detected in polar bears at 414.8 ng/g lipid weight, more than 30 times its concentration in primary prey (ringed seal). **TBPH** was not detected in polar bears.

Estimated BAFs for the possible microbial degradation and/or hydrolysis products tetrabromophthalic acid and tetrabromobenzoic acid are below numerical thresholds for bioaccumulation concern; i.e. they are formally B1 (Table 1-3). However, it should be noted that for the benzoic acid the calculated BAF for upper trophic-level fish is close to the B2 criterion (i.e. log BAF = 3.00). Without metabolism, the predicted log BAF is 5.18, which exceeds the threshold for high concern (B3). Based on the above results this expected chief degradation product of **TBB** is considered to have moderate bioaccumulation potential (B2). This is appropriate also because this substance is judged likely to be much more persistent in the environment than the parent, thus increasing its potential to reach and accumulate in organisms.

There are no experimental data for 3,4,5,6-tetrabromo-1,2-benzenedicarboxylic acid, mixed esters with diethylene glycol and propylene glycol (CASRN 77098-07-8 and 20566-35-2), but based on chemical structure and estimated BCF and BAF (Table 1-3), bioaccumulation potential is considered low (B1) for the parent substance. Bioaccumulation potential is also judged to be low for all potential hydrolysis products.

Similarly there are no experimental bioaccumulation data for 1,2-(2,3-dibromopropyl) benzene dicarboxylate (CASRN 7415-86-3). Both estimated BCF and BAF (the latter with metabolism included) miss the threshold for moderate concern (log=3; Table 1-3), although the regression-based log BCF is close to the concern level. With metabolism excluded, the predicted log BAF exceeds the threshold for high concern (B3). Based on these results, 1,2-(2,3-dibromopropyl) benzene dicarboxylate (CASRN 7415-86-3) is judged to have moderate bioaccumulation potential (B2).

Table 1-3: Environmental Fate Data for the Brominated Phthalates Cluster

Property	Brominated Phthalate Cluster Members				
Chemical Name	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1,2-bis(2-ethylhexyl) ester ¹	Benzoic acid, 2,3,4,5-tetrabromo-, 2-ethylhexyl ester	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1-[2-(2-hydroxyethoxy)ethyl] 2-(2-hydroxypropyl) ester ⁴	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	1,2-Benzenedicarboxylic acid, 1,2-bis(2,3-dibromopropyl) ester
CASRN	26040-51-7	183658-27-7	20566-35-2	77098-07-8	7415-86-3
Photooxidation Half-life	5.8 hours (estimated) ²	11.7 hours (estimated) ²	4.2 hours (estimated) ²	See 20566-35-2	5.8 hours (estimated) ²
Hydrolysis Half-life	pH 7 = 29 days (estimated) ² ; pH 8 = 2.9 days (estimated)²	pH 7 = 34 days (estimated) ² ; pH 8 = 3.4 days (estimated) ²	pH 7 = 7.9 days (estimated) ² ; pH 8 = 19 hours (estimated) ²	See 20566-35-2	pH 7 = 315 days (estimated) ² ; pH 8 = 31.5 days (estimated) ²
Biodegradation (ready biodegradation test data; see text for additional information)	<4% biodegradation after 28 day (not readily biodegradable) ^{1,3}	No data 6% in 28 days in 301D (BFR database, confidential data, described as adequate guideline study)	No Data	See 20566-35-2	No Data
Bioconcentration Factor	Log BCF = 1.1 (estimated) ² 1.7-6.2 (not log; BFR database, confidential data, described as adequate guideline study)	Log BCF = 3.27 (estimated) ²	Log BCF = 1.94 (estimated) ²	See 20566-35-2	Log BCF = 2.87 (estimated) ²
Bioaccumulation Factor⁵	Log BAF = 0.38 (estimated) ²	Log BAF = 3.32 (estimated) ²	Log BAF = 0.82 (estimated) ²	See 20566-35-2	Log BAF = 1.10 (estimated) ² Log BAF = 4.79 (estimated; without metabolism)
Log K_{oc}	5.9 (estimated, MCI method) ² 7.4 (estimated, log Kow method) ²	4.5 (estimated, MCI method) ² 5.7 (estimated, log Kow method) ²	1.0 (estimated, MCI method) ² 2.0 (estimated, log Kow method) ²	See 20566-35-2	3.5 (estimated, MCI method) ² 3.5 (estimated, log Kow method) ²
Henry's Law Constant (atm-m³/mol)	3.1×10 ⁻⁷ (estimated, group estimate) ²	7.1×10 ⁻⁶ (estimated, group estimate) ²	2.2×10 ⁻²¹ (estimated, group estimate) ²	See 20566-35-2	2.8×10 ⁻¹⁴ (estimated, group estimate) ²

Property	Brominated Phthalate Cluster Members				
Chemical Name	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1,2-bis(2-ethylhexyl) ester ¹	Benzoic acid, 2,3,4,5-tetrabromo-, 2-ethylhexyl ester	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, 1-[2-(2-hydroxyethoxy)ethyl] 2-(2-hydroxypropyl) ester ⁴	1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrabromo-, mixed esters with diethylene glycol and propylene glycol	1,2-Benzenedicarboxylic acid, 1,2-bis(2,3-dibromopropyl) ester
Fugacity (Level III Model)²				See 20566-35-2	
Air (%)	0.169	0.319	0.001		0.00000066
Water (%)	11.6	11.8	37		11.1
Soil (%)	88.2	86.9	62.9		87
Sediment (%)	<0.1	0.95	0.09		1.9

¹ Brominated Phthalate Ester Panel (BR PEP) American Chemistry Council. August 5, 2004. Revised Robust Summary and Test Plan for Phthalic Acid Tetrabromo Bis 2-Ethylhexyl Ester (CASRN 26040-51-7). Prepared by Health & Environmental Horizons, Ltd. Available online from: <http://www.epa.gov/hpv/pubs/summaries/phthacid/c15484tc.htm> as of June 23, 2010.

² EPA. 2012. Estimation Programs Interface Suite™ for Microsoft® Windows, v4.11. Environmental Protection Agency, Washington, DC, USA. Available online from: <http://www.epa.gov/opptintr/exposure/pubs/episuitedi.htm>.

³ Test substance used in the biodegradation study is indicated by the sponsor as Pyronil 45 with a purity of 95%.

⁴ ECHA: <http://apps.echa.europa.eu/registered/data/dossiers/DISS-9ea569d1-072b-18ab-e044-00144f67d031/DISS-9ea569d1-072b-18ab-e044-00144f67d031> DISS-9ea569d1-072b-18ab-e044-00144f67d031.html ; — indicates no data or no reliable data for this endpoint

⁵ Estimated upper trophic log BAF from the BCFBAF program (in Estimation Programs Interface Suite™ for Microsoft® Windows, v4.11; see footnote 2. Estimates include metabolism except as noted.

1.3 ENVIRONMENTAL FATE and BIOACCUMULATION – DATA NEEDS

1.3.1 Ambient Environment

Very little information exists on the environmental fate and bioaccumulation of the Brominated Phthalates Cluster (BPC) members, and what data do exist, are for **TBPH** and **TBB** only.

Therefore, comprehensive studies are needed for many endpoints and for all cluster members. All cluster members should be tested individually and all major degradation products should be quantified. This means that it is necessary to test **TBB** and **TBPH** separately. There is no point in testing using standard ready or inherent biodegradability tests. Among published guidelines, only simulation tests such as OECD TG 307 (aerobic and anaerobic soil transformation) and OECD TG 308 (aerobic and anaerobic transformation in aquatic sediment) are likely to yield information useful for informing environmental exposure (therefore, risk) assessment. Based on photodegradation studies of **TBPH** and **TBB** using organic solvents, cluster members may undergo direct photolysis; however additional work is needed to confirm this. These studies should measure rates and products under relevant conditions (i.e. with water as solvent). In

addition, to provide needed information on key environmentally important physical properties, Henry's Law constant, Koc and Koa should be determined experimentally using standard protocols and under GLP conditions. Comprehensive bioaccumulation studies are needed for all BPC cluster members, and these should include several aquatic and terrestrial species selected from organisms commonly used in bioaccumulation testing. Specialized protocols are available for some of the above endpoints and may be adapted for BPC members; e.g. the aerobic/ anaerobic sediment testing methodology developed for decaBDE under the PBDE SNUR.

1.3.2 Indoor Environment

It is EPA's judgment that exposure via dust may be important, yet little information is available on how these compounds get into house dust. This process may involve direct transfer from flame-retarded objects, driven by partitioning properties of the Brominated Phthalates Cluster (BPC) substances. To better understand these processes, and therefore more accurately assess indoor exposure, it is necessary to conduct studies to determine rates of migration of cluster members from flame-retarded indoor objects; and rates and mechanisms of partitioning into dust and any other media that may be vectors for human exposure.

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