Chemosphere xxx (2014) xxx–xxx

Contents lists available at ScienceDirect

Chemosphere

journal homepage: www.elsevier.com/locate/chemosphere

Assessing the persistence, bioaccumulation potential and toxicity of brominated flame retardants: Data availability and quality for 36 alternative brominated flame retardants

Greta Stieger, Martin Scheringer *, Carla A. Ng, Konrad Hungerbühler

Institute for Chemical and Bioengineering, ETH Zürich, 8093 Zürich, Switzerland

ARTICLE INFO

Article history:
Received 14 October 2013
Received in revised form 11 January 2014
Accepted 15 January 2014
Available online xxxx

Keywords:
Brominated flame retardants
PBT assessment
Baseline toxicity
Octanol–water partition coefficient

ABSTRACT

Polybrominated diphenylethers (PBDEs) and hexabromocyclododecane (HBCDD) are major brominated flame retardants (BFRs) that are now banned or under restrictions in many countries because of their persistence, bioaccumulation potential and toxicity (PBT properties). However, there is a wide range of alternative BFRs, such as decabromodiphenyl ethane and tribromophenol, that are increasingly used as replacements, but which may possess similar hazardous properties. This necessitates hazard and risk assessments of these compounds. For a set of 36 alternative BFRs, we searched 25 databases for chemical property data that are needed as input for a PBT assessment. These properties are degradation half-life, bioconcentration factor (BCF), octanol–water partition coefficient (K_{ow}), and toxic effect concentrations in aquatic organisms. For 17 of the 36 substances, no data at all were found for these properties. Too few persistence data were available to even assess the quality of these data in a systematic way. The available data for K_{ow} and toxicity show surprisingly high variability, which makes it difficult to identify the most reliable values. We propose methods for systematic evaluations of PBT-related chemical property data that should be performed before data are included in publicly available databases. Using these methods, we evaluated the data for K_{ow} and toxicity in more detail and identified several inaccurate values. For most of the 36 alternative BFRs, the amount and the quality of the PBT-related property data need to be improved before reliable hazard and risk assessments of these substances can be performed.

© 2014 Elsevier Ltd. All rights reserved.

1. Introduction

Brominated flame retardants (BFRs) comprise a wide range of brominated aromatic and aliphatic compounds (Bergman et al. 2012). Two types of BFRs widely used in the last decades are polybrominated diphenylethers (PBDEs) and hexabromocyclododecane (HBCDD). Because of their hazardous properties regarding persistence, bioaccumulation potential and toxicity (PBT properties), the use of these substances is now restricted or prohibited under various national and international legislations (UNEP, 2013; ECHA, 2013a). However, PBDEs and HBCDD are often replaced by other BFRs such as decabromodiphenyl ethane, pentabromotoluene, pentabromoethylbenzene, and many more. Often, the chemical properties of these substitutes are only poorly known; thus concerns about their PBT characteristics remain (Covaci et al., 2011).

PBT assessment is a component of chemicals assessment that focuses on three hazardous properties of organic chemicals. These properties include persistence (P), potential for bioconcentration and bioaccumulation (B), and aquatic toxicity (T); Strempel et al. (2012) provide an overview of several PBT assessment schemes. Data required for a PBT assessment include degradation half-lives in water or soil for P, octanol–water partition coefficients, bioconcentration and, in some cases, also bioaccumulation factors for B, and toxic effect concentrations from chronic toxicity tests or, if no chronic toxicity data are available, acute tests for T (Strempel et al., 2012).

Here we evaluate the availability and quality of chemical property data that are needed for a PBT assessment of alternative BFRs. We selected 36 BFRs that were listed by Bergman et al. (2012) and also found in the PBT database compiled by Strempel et al. (2012). To retrieve chemical property data for these chemicals, we extensively searched 25 publicly accessible databases. On this basis, we analyze the number of data points for each property and chemical, discuss the variability and scatter in the data, and evaluate the data for the octanol–water partition coefficient (K_{ow}) and the aquatic toxicity in more detail.

* Corresponding author. Tel.: +41 44 632 3062; fax: +41 44 632 1189.
E-mail address: scheringer@chem.ethz.ch (M. Scheringer).

http://dx.doi.org/10.1016/j.chemosphere.2014.01.083
0045-6535/© 2014 Elsevier Ltd. All rights reserved.

Please cite this article in press as: Stieger, G., et al. Assessing the persistence, bioaccumulation potential and toxicity of brominated flame retardants: Data availability and quality for 36 alternative brominated flame retardants. Chemosphere (2014), http://dx.doi.org/10.1016/j.chemosphere.2014.01.083

2. Materials and methods

The BFRs investigated are listed in Table 1, which is based on information from Bergman et al. (2012). For these 36 chemicals we retrieved chemical property data from 25 publicly accessible databases, including the database of the European Chemicals Agency (ECHA), http://www.echa.eu; and the OECD eChemPortal, which provides links to 24 participating data sources, http://www.echemportal.org. The property data include biodegradation half-life in soil, $t_{1/2,soil}$, for persistence, the octanol–water partition coefficient, K_{ow}, and the bioconcentration factor, BCF, for bioaccumulation, and chronic and acute effect concentrations, Tc and Ta, for aquatic organisms (algae, daphnia, fish) for toxicity. The databases were searched by CAS number for each of the 36 BFRs and all available data entries for the PBT properties, including both experimental and estimated values, were collected and stored. The data were retrieved in November and December 2012.

We determined the numbers of data points that were found for each chemical and property. For chemicals with several data points per property (Ta, BCF, K_{ow}), we plotted the data in order to visualize the variability of the data. For the K_{ow} and toxicity data in particular, we evaluated the plausibility of individual data points.

The K_{ow} of organic chemicals is largely determined by the chemicals' solubility in water, S_w (Schwarzenbach et al., 2003). S_w is determined by the energy that is required to accommodate the solute in water, i.e. to break hydrogen bonds between water molecules and form a cavity that can take up the solute molecule. For neutral or weakly polar organic chemicals, this amount of energy is directly proportional to the molecular weight. In the case of polychlorinated biphenyls (PCBs), $\log K_{ow}$ follows a highly significant positive linear relationship with increasing degree of chlorination and thus increasing molecular weight (Schenker et al., 2005). Many brominated aromatic compounds in our set are also non-ionizing organic substances; for substances with phenolic groups, the K_{ow} is measured at sufficiently low pH where ionization is suppressed and the substances are predominantly present in their neutral form (Sotomatsu et al., 1993; Kuramochi et al., 2004). Therefore, we expect that a similar relationship can be derived for the brominated aromatic substances in our set of 36 alternative BFRs.

To establish this relationship, we looked for series of compounds with similar aromatic backbones, in analogy to the set of PCB congeners. From the set of 36 BFRs, two such subsets were available: (i) 14 monoaromatic BFRs and (ii) 9 di-aromatic structures, including TBBPA, 6 TBBPA derivatives, as well as DBDPE and BTBPE. Together, these two sets include 23 of the 36 BFRs. Because K_{ow} values were available for only 11 of these 23 substances, we included the $\log K_{ow}$ values collected by Strempel et al. (2012) and Bergman et al. (2012) in our analysis. Because the $\log K_{ow}$ values for these 23 compounds showed a high degree of variability, we implemented a two-step process to find the best relationship between $\log K_{ow}$ and molecular weight. First, we used all of the $\log K_{ow}$ data to derive a linear relationship with molecular weight. We then used this linear relationship to determine, for each substance, which $\log K_{ow}$ values seemed implausible because they were either too low or too high. In general, for chemicals where the variability of the K_{ow} data was high, the lower $\log K_{ow}$ values were (much) below the linear relationship whereas most of the higher ones were in line with it. In the second step, we excluded those $\log K_{ow}$ values that were clearly below or above the linear relationship and calculated for each chemical the "best guess" $\log K_{ow}$ as the average of the remaining $\log K_{ow}$ values (these "best guess" estimates are the data points shown in Fig. 1, left).

Table 1
CAS numbers, common names, and practical abbreviations proposed by Bergman et al. (2012) of the 36 BFRs investigated in this work.

Count	CAS number	Common name	Practical abbreviation
1	79-94-7	Tetrabromobisphenol A	TBBPA
2	632-79-1	3,4,5,6-Tetrabromophthalic anhydride	TEBP-Anh
3	52434-90-9	1,3,5-Tris(2,3-dibromopropyl)-1,3,5-triazine-2,4,6-trione	TDBP-TAZTO
4	66710-97-2	Tetrabromobisphenol A bis(2-hydroxyethyl)ether bisacrylate	TBBPA-BHEEBA
5	59447-55-1	Pentabromobenzyl acrylate	PBB-Acr
6	34571-16-9	1,2,3,4,7,7-Hexachloro-5-(2,3,4,5-tetrabromophenyl)-bicyclo[2.2.1]hept-2-ene	HCTBPH
7	26040-51-7	Bis(2-ethylhexyl) tetrabromophthalate	BEH-TEBP
8	39635-79-5	Tetrabromobisphenol S	TBBPS
9	32588-76-4	N,N′-Ethylenebis (tetrabromophthalimide)	EBTEBPI
10	38521-51-6	Pentabromobenzyl bromide	PBBB
11	20566-35-2	2-(2-Hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromophthalate	HEEHP-TEBP
12	87-82-1	Hexabromobenzene	HBB
13	3194-57-8	1,2,5,6-Tetrabromo-cyclooctane	TBCO
14	3278-89-5	2,4,6-Tribromophenyl allyl ether	TBP-AE
15	25327-89-3	Tetrabromobisphenol A bis(allyl) ether	TBBPA-BAE
16	21850-44-2	Tetrabromobisphenol A bis(2,3-dibromopropyl) ether	TBBPA-BDBPE
17	87-83-2	Pentabromotoluene	PBT
18	3296-90-0	Dibromoneopentyl glycol	DBNPB
19	3322-93-8	4-(1,2-Dibromoethyl)-1,2-dibromocyclohexane	DBE-DBCH
20	85-22-3	Pentabromoethylbenzene	PBEB
21	25713-60-4	Tris(2,4,6-tribromophenoxy)-s-triazine	TTBP-TAZ
22	37853-59-1	1,2-Bis(2,4,6-tribromophenoxy)ethane	BTBPE
23	84852-53-9	Decabromodiphenyl ethane	DBDPE
24	615-58-7	2,4-Dibromophenol	DBP
25	35109-60-5	2,4,6-Tribromophenyl 2,3-dibromopropyl ether	TBP-DBPE
26	37853-61-5	Tetrabromobisphenol A bismethyl ether	TBBPA-BME
27	33798-02-6	3,3′,5,5′-Tetrabromobisphenol A bisacetate	TBBPA-BOAc
28	3555-11-1	Pentabromophenol allyl ether	PBP-AE
29	126-72-7	Tris(2,3-dibromopropyl) phosphate	TDBPP
30	4162-45-2	Tetrabromobisphenol A bis(2-hydroxyethyl) ether	TBBPA-BHEE
31	42757-55-1	Tetrabromobisphenol S bis(2,3-dibromopropyl ether)	TBBPS-BDBPE
32	23488-38-2	1,2,4,5-Tetrabromo-3,6-dimethylbenzene	TBX
33	608-71-9	Pentabromophenol	PBP
34	51936-55-1	5,6-Dibromo-1,10,11,12,13,13-hexachloro-11-tricyclo[8.2.1.02,9]tridecene	DBHCTD
35	118-79-6	2,4,6-Tribromophenol	TBP
36	39569-21-6	2,3,4,5-Tetrabromo-6-chlorotoluene	TBCT

Please cite this article in press as: Stieger, G., et al. Assessing the persistence, bioaccumulation potential and toxicity of brominated flame retardants: Data availability and quality for 36 alternative brominated flame retardants. Chemosphere (2014), http://dx.doi.org/10.1016/j.chemosphere.2014.01.083

Download English Version:

https://daneshyari.com/en/article/6308703

Download Persian Version:

https://daneshyari.com/article/6308703

Daneshyari.com