

Evaluation of small brominated alkyl alcohols for a possible RoHS restriction

Background document

September 2016

Substance Name: Small brominated alkyl alcohols (group)

EC Number(s): 202-480-9; 202-489-8; 243-029-6; 627-179-3; 221-967-7; 622-370-8; 253-057-0; further substances not associated with EC numbers detailed in Appendix I

CAS Number(s): 96-13-9; 96-21-9; 106023-63-6; 19398-47-1; 4021-75-4; 14396-65-7; 855236-37-2; 87018-38-0; 105100-80-9; 213821-22-8; 408319-76-6; 159475-15-7; 343268-04-2; 76377-07-6; 59287-66-0; 856991-78-1; 100606-66-4; 213821-20-6; 98069-26-2; 3296-90-0; 44804-46-8; 1522-92-5; 36483-57-5; further substances not associated with CAS numbers detailed in Appendix I

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Abbreviations

| | |
|----------|--|
| BFR | Brominated flame retardant |
| CLP | Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006 (REACH) |
| DEPA | Danish Environmental Protection Agency |
| DTU Food | Danish Technical University, National Food Institute |
| EEE | Electrical and electronic equipment |
| EFRA | The European Flame Retardant Association |
| MSDS | Material safety data sheet |
| n.d. | Not defined |
| SBAA | Small brominated alkyl alcohols |
| SME | Small and medium enterprises |

Background

Hazardous substances in electrical and electronic equipment (EEE) are regulated by the RoHS Directive 2011/65/EU (RoHS 2). According to article 6(1) it is possible for member states to submit a proposal for adding new substances to the list of restricted substances of the directive. Article 6(1) and 6(2) describe the criteria and requirements for proposals for restrictions respectively.

In 2014 the Danish EPA performed a survey on brominated flame retardants (BFRs) (DEPA 2014). On the basis of its results, the Danish Technical University (DTU Food) investigated possibilities of grouping BFRs. One of the groupings; the small linear and branched brominated alkyl alcohols, including 2,3-dibromo-1-propanol (CAS 96-13-9) and 2,2-bis(bromomethyl)propane-1,3-diol (CAS 3296-90-0) and 2,2-bis-(bromomethyl)-3-bromo-1-propanol (CAS 36483-57-5), was chosen for further investigation and the grouping was extended to include also theoretical compounds. The category, defined as having 3-5 carbons, 2-3 bromine atoms and 1-2 alcohol groups, comprises 62 members. (DEPA 2016)

Thus, following a tender process, the Danish EPA has commissioned Oeko-Institut e.V along with COWI AS, a project to collect, assess and present scientific data to support a proposal for restriction of small brominated alkyl alcohol in the RoHS Directive, if the data prove to be adequate.

Data has been compiled based on publicly available data. The following background document has been prepared to support collection of further data through an online stakeholder consultation. Stakeholders are asked to provide input and may use the stakeholder questionnaire as guidance as to possible areas of interest for contributing further information and data¹. Following this stage, an evaluation shall be performed and if relevant, a dossier shall be prepared recommending a restriction of this BFR group under the RoHS Directive.

¹ See questionnaire available on the consultation page under: <http://rohs.exemptions.oeko.info/index.php?id=212>

1. Identification, Classification and Labelling, Legal Status and Use Restrictions

1.1. Identification

The group of substances is defined as small brominated linear and branched alkyl alcohols with 3-5 carbons, 1-2 alcohol groups, and 2-4 bromine atoms. In the identified group the smallest member has 3 carbons, two bromine atoms and one alcohol group, such as 2,3-dibromo-1-propanol (CAS 96-13-9), and the two largest members have 5 carbons, 2-3 bromine atoms and 1-2 alcohol groups (2,2-bis(bromomethyl)propane-1,3-diol, CAS 3296-90-0 and 2,2-bis-(bromomethyl)-3-bromo-1-propanol, CAS 36483-57-5).

According to the DEPA report (2016), the substance group theoretically² comprises 62 members. Two substances are structurally identical but with different CAS numbers. CAS numbers have been allocated to 22 of the members. For seven of the substances, EC numbers exist. The general substance identity and composition of the various group substances is presented in Table 1-1. More detailed information is provided for substances with both CAS and EC number in Table 1-2. For 14 substances there was lacking information on substance identity, they are compiled separately in Table 1-3.

A complete list of all 62 substances understood to fall in scope of the proposed group is available in Appendix I. This list is reproduced on the basis of the data available in the DEPA (2016) report. It is understood that some of the substances may be theoretical.

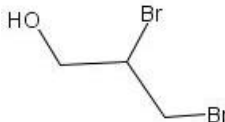
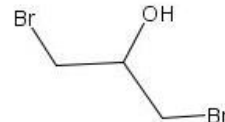
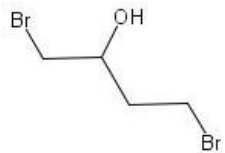
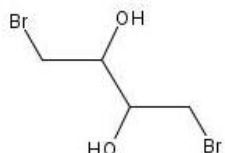
1.1.1. Name, other identifiers, and composition of the substance

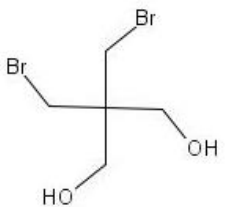
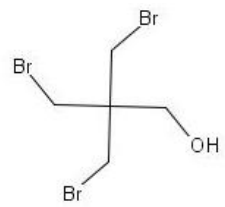
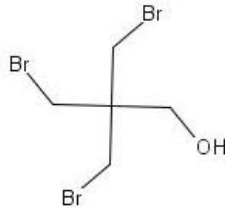
Table 1-1: Substance identity and composition

| Chemical name | Small brominated alkyl alcohols (substance group) |
|------------------------|--|
| EC number | 202-480-9; 202-489-8; 243-029-6; 627-179-3; 221-967-7; 622-370-8; 253-057-0 |
| CAS number | 96-13-9; 96-21-9; 106023-63-6; 19398-47-1; 4021-75-4; 14396-65-7; 855236-37-2; 87018-38-0; 105100-80-9; 213821-22-8; 408319-76-6; 159475-15-7; 343268-04-2; 76377-07-6; 59287-66-0; 856991-78-1; 100606-66-4; 213821-20-6; 98069-26-2; 3296-90-0; 44804-46-8; 1522-92-5; 36483-57-5; further substances not associated with CAS numbers are detailed in Appendix I |
| Molecular formula | $C_xBr_yO_z$; $x=3-5$; $y=2-4$; $z=1-2$ |
| Molecular weight range | 217.9-324.8 (where data available) |

² The DEPA report (2016) identified the chemical structures of the theoretical members of the category and generated SMILES codes.

Table 1-2: Substance identity and composition

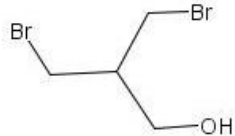
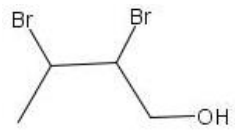
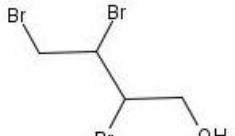
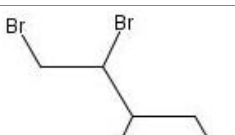
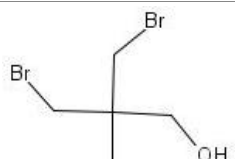
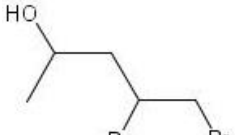
| Chemical name | EC number | CAS number | IUPAC name | Index no. in Annex VI of the CLP Regulation | Molecular formula | Molecular weight | Synonyms | Structural formula | Degree of purity |
|----------------------------|-----------|------------|--|---|--|------------------|---|---|------------------|
| 2,3-Dibromo-1-propanol | 202-480-9 | 96-13-9 | 2,3-Dibromo-propan-1-ol; 2,3-Dibromo-1-propanol | 602-088-00-1 | C ₃ H ₆ Br ₂ O | 217.9 | 2,3-dibromopropan-1-ol; DBP; DBP (flame retardant); 1,2-dibromopropan-3-ol; 2,3-dibromopropyl alcohol |  | |
| 1,3-dibromopropan-2-ol | 202-489-8 | 96-21-9 | 1,3-Dibromo-propan-2-ol | n.d. | C ₃ H ₆ Br ₂ O | 217.9 | 1,3-Dibromo-2-hydroxypropane; 1,3-Dibromo-2-propanol; 1,3-Dibromohydrin; 1,3-Dibromopropanol; 2-Hydroxy-1,3-dibromopropane; Glycerol 1,3-dibromohydrin; Glycerol a,g-dibromohydrin; NSC 636; a,g-Dibromohydrin; a-Dibromohydrin |  | |
| 1,4-dibromobutan-2-ol | 243-029-6 | 19398-47-1 | 1,4-dibromo-butan-2-ol | n.d. | C ₄ H ₈ Br ₂ O | 231.9 | - |  | |
| 1,4-Dibromo-2,3-butanediol | 627-179-3 | 14396-65-7 | 1,4-Dibromo-2,3-butanediol | n.d. | C ₄ H ₈ Br ₂ O ₂ | 247.9 | |  | |

| Chemical name | EC number | CAS number | IUPAC name | Index no. in Annex VI of the CLP Regulation | Molecular formula | Molecular weight | Synonyms | Structural formula | Degree of purity |
|---|-----------|------------|---|---|--------------------|------------------|---|--|------------------|
| 2,2-bis(bromomethyl)propane-1,3-diol | 221-967-7 | 3296-90-0 | 2,2-Bis(bromomethyl)-1,3-propanediol 2,2-Bis(bromomethyl)propane-1,3 2,2-Bis(bromomethyl)propane-1,3-diol FR-522 | n.d. | $C_5H_{10}Br_2O_2$ | 262.0 | Dibromo-neopentyl-glycol, 2,2-Bis(bromomethyl)-1,3-propanediol (Technical Grade) |  | |
| 3-Bromo-2,2-bis(bromomethyl)-1-propanol | 622-370-8 | 1522-92-5 | 3-Bromo-2,2-bis(bromomethyl)-1-propanol Pentaerythritol Tribromide | n.d. | $C_5H_9Br_3O$ | 324.8 | - |  | |
| 2,2-dimethylpropan-1-ol (TBNPA) | 253-057-0 | 36483-57-5 | 2,2-Dimethylpropan-1-ol, tribromo derivative 3,3,3-tribromo-2,2-dimethylpropan-1-ol FR-513 | n.d. | $C_5H_9Br_3O$ | 324.8 | 2,2-dimethylpropan-1-ol, tribromo derivative* Trisbromoneopentyl alcohol, Tribromoneopentanol; 2,2-Bis-(bromomethyl)-3-bromo-1-propanol; tribromoneopentyl alcohol |  | |

There are several substances in this group for which EC numbers are not available and further information on identity, such as chemical name is lacking. The lack of records in databases such as the ECHA Information on Chemicals database, The OECD's eChemPortal and the industry supplier's database, LookChem, gives an impression that the substances might not be available on the market.

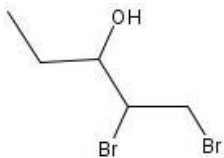
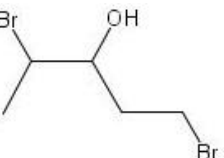
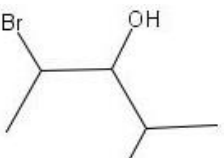
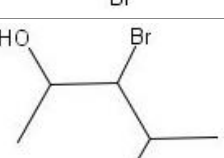
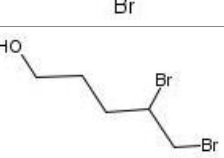
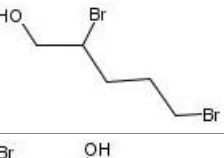
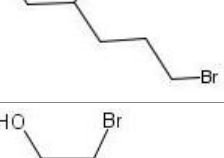

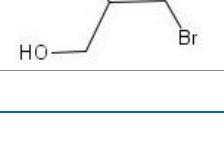
3-Bromo-2,2-bis(bromomethyl)-1-propanol (CAS 1522-92-5) and 2,2-dimethylpropan-1-ol (CAS 36483-57-5) have an identical structural formula. Therefore DEPA (2016) considered them as a single substance; Lassen et al. (2014) also refer to these two substance as the same substance. However, they have different EC numbers and the ECHA Information on Chemicals database lists two different entries. Reports such as e.g. EFSA (2012) refer to only one CAS number.

Table 1-3: SBAA with lacking information on substance identity and composition

| Chemical name | CAS number | Molecular formula | Structural formula | Remarks |
|------------------------------------|-------------|--|--|--|
| 3-Bromo-2-(bromomethyl)-1-propanol | 106023-63-6 | C ₄ H ₈ Br ₂ O |  | No results in ECHA database and eChemPortal; however supplier are available according to LookChem ³ |
| 2,3-dibromobutan-1-ol | 4021-75-4 | C ₄ H ₈ Br ₂ O |  | No results in ECHA database and eChemPortal; however supplier are available according to LookChem ⁴ |
| 2,3,4-Tribromo-1-butanol | 855236-37-2 | C ₄ H ₇ Br ₃ O |  | No results in ECHA database, eChemPortal and LookChem |
| 1,2,4-Tribromo-3-butanol | 87018-38-0 | C ₄ H ₇ Br ₃ O |  | |
| 2,2-Bis(bromomethyl)-1-propanol | 105100-80-9 | C ₅ H ₁₀ Br ₂ O |  | |
| 4,5-Dibromo-2-pentanol | 213821-22-8 | C ₅ H ₁₀ Br ₂ O |  | |

³ <http://www.lookchem.com/newsell/search.aspx?key=106023-63-6>

⁴ <http://www.lookchem.com/newsell/search.aspx?key=4021-75-4>

| Chemical name | CAS number | Molecular formula | Structural formula | Remarks |
|--|-------------|--|--|--|
| 1,2-Dibromo-3-pentanol | 408319-76-6 | C ₅ H ₁₀ Br ₂ O |  | |
| 1,4-dibromo-(R*,R*)-(9CI)-3-pentanol | 159475-15-7 | C ₅ H ₁₀ Br ₂ O |  | |
| 2,4-Dibromo-3-pentanol | 343268-04-2 | C ₅ H ₁₀ Br ₂ O |  | |
| 3,4-Dibromo-(2R*,3S*,4S*)-(9CI)-2-pentanol | 76377-07-6 | C ₅ H ₁₀ Br ₂ O |  | |
| 4,5-Dibromo-1-pentanol | 59287-66-0 | C ₅ H ₁₀ Br ₂ O |  | |
| 2,5-Dibromo-1-pentanol | 856991-78-1 | C ₅ H ₁₀ Br ₂ O |  | |
| 2-Pentanol, 1,5-dibromo- | 100606-66-4 | C ₅ H ₁₀ Br ₂ O |  | No results in ECHA database and eChemPortal; however supplier are available according to LookChem ⁵ |
| 2,5-Dibromo-2-pentanol | 213821-20-6 | C ₅ H ₁₀ Br ₂ O |  | No results in ECHA database, eChemPortal and LookChem |
| 4-Bromo-2-(bromomethyl)-1-butanol | 98069-26-2 | C ₅ H ₁₀ Br ₂ O |  | |

⁵ <http://www.lookchem.com/newsell/search.aspx?key=100606-66-4>

1.1.2. Physico-chemical properties

Physico-chemical properties are summarised for the group in Table 1-4 below, where data is available for at least 3 substances (i.e. suggesting a range). Table 1-5 provides the data available for specific substances.

Table 1-4: Overview of physico-chemical properties of SBAA

| Property | Value |
|--|--|
| Physical state at 20°C and 101.3 kPa | Variable (liquid/solid) |
| Melting/freezing point | Range: 8°C – 109.5 °C |
| Boiling point | 83 °C – 365.3 °C |
| Vapour pressure | Data available only for two substances |
| Water solubility | Variable (insoluble – very soluble) |
| Partition coefficient n-octanol/water (log P _{OW}) | Range: 0.96 – 2.6 |
| Dissociation constant | Data available only for one substance |
| Vapour density relative to air | Data available only for one substance |
| Specific gravity | Data available only for one substance |

Table 1-5: Overview of physico-chemical properties

| Substance (CAS) | Physical state at 20°C and 101.3 kPa | Melting/freezing point | Boiling point | Vapour pressure | Water solubility | Partition coefficient n-octanol/ water (log P _{ow}) | Dissociation constant | Vapour density relative to air | Specific gravity | Sources |
|---|--------------------------------------|------------------------|-----------------------|--|--|---|-----------------------|--------------------------------|------------------|--|
| 2,3-Dibromo-1-propanol (CAS 96-13-9) | Clear colourless liquid | 8°C | 219°C | 0.09 mm Hg at 25°C | 52 g/L at 25°C | 0.96 | | 2.12 | 2.12 at 20°C/4°C | TOXNET ChemIDplus ⁶ |
| 1,3-dibromopropan-2-ol (CAS 96-21-9) | - | - | 83 °C * 194.3°C ** | - | - | - | - | - | - | *: GESTIS Stoffdatenbank ⁷ **: LookChem ⁸ |
| 1,4-dibromobutan-2-ol (CAS 19398-47-1) | Brown viscous liquid. | - | 220.1 °C | - | - | - | - | - | - | LookChem ⁹ |
| 1,4-Dibromo-2,3-butanediol (CAS 14396-65-7) | Solid | 82-84 °C | 365.3°C | - | - | - | - | - | - | LookChem ¹⁰ |
| 2,2-bis(bromomethyl)propane-1,3-diol (CAS 3296-90-0) | Solid | 108.5 - 109.5 °C | ca. 270°C | 1x10 ⁻³ to 4.1 x 10 ⁻³ Pa at 25 °C, mean=2x10 ⁻³ Pa | Very soluble: 19.4 g/l at 20.0 ± 0.5°C | 1.08 | - | - | - | ECHA registration dossier ¹¹ |
| 3-Bromo-2,2-bis(bromomethyl)-1-propanol (CAS 1522-92-5) | Solid | 64-66 °C | 365.3°C | - | Insoluble | - | - | - | - | LookChem ¹² |

⁶ <https://chem.sis.nlm.nih.gov/chemidplus/rn/96-13-9#physical>⁷ <http://gestis.itrust.de/nxt/gateway.dll?f=templates&fn=default.htm&vid=gestisdeu:sdbdeu>⁸ <http://www.lookchem.com/newsell/search.aspx?key=96-21-9>⁹ <http://www.lookchem.com/newsell/search.aspx?key=19398-47-1>¹⁰ <http://www.lookchem.com/newsell/search.aspx?key=14396-65-7>¹¹ <https://echa.europa.eu/registration-dossier/-/registered-dossier/7873/1>¹² <http://www.lookchem.com/newsell/search.aspx?key=1522-92-5>

| Substance (CAS) | Physical state at 20°C and 101.3 kPa | Melting/freezing point | Boiling point | Vapour pressure | Water solubility | Partition coefficient n-octanol/ water (log P _{ow}) | Dissociation constant | Vapour density relative to air | Specific gravity | Sources |
|---|--------------------------------------|------------------------|---------------|-----------------|-------------------------------|---|-----------------------|--------------------------------|------------------|---|
| 2,2-dimethylpropan-1-ol (TBNPA) (CAS 36483-57-5) | Solid** | 68,96°C* | 145°C* | - | Soluble: 1.93 g/l at 20.1°C** | 2.6 ** | - | - | - | * GESTIS Stoffdatenbank; ** ECHA registration dossiers |

1.2. Classification and labelling status

The Classification, Labelling and Packaging (CLP) regulation¹³ ensures that the hazards presented by chemicals are clearly communicated to workers and consumers in the European Union through classification and labelling of chemicals. Annex VI of Regulation No 1272/2008 lists substances where a harmonized classification exists based on e.g. human health concerns. However, mostly, suppliers decide independently as to the classification of a substance or mixture, which is then referred to as self-classification.

Classification in Annex VI Regulation No 1272/2008

A harmonized classification according to Annex VI Regulation No 1272/2008 is available for one substance: 2,3-dibromopropan-1-ol (CAS 96-13-9), the classification according to Table 3.1 of Annex VI is presented in Table 1-6.

Table 1-6: Classification according to part 3 of Annex VI, Table 3.1 (list of harmonized classification and labelling of hazardous substances) of Regulation (EC) No 1272/2008

| Index No. | International Chemical ID | EC No. | CAS No. | Classification | | Labelling | | | Spec. Conc. Limits, M-factors | Notes |
|--------------|---|-----------|---------|--|---|--------------------------------|---|---------------------------------|-------------------------------|-------|
| | | | | Hazard Class and Category Code(s) | Hazard statement code(s) | Pictogram, Signal Word Code(s) | Hazard statement code(s) | Suppl. Hazard statement code(s) | | |
| 602-088-00-1 | 2,3-dibromopropan-1-ol; 2,3-dibromo-1-propanol | 202-480-9 | 96-13-9 | Carc. 1B Repr. 2 Acute Tox. 3 Acute Tox. 4 Acute Tox. 4 Aquatic Chronic 3 | H350 H361f H311 H332 H302 H412 | GHS08 GHS07 Dgr | H350 H361f H311 H332 H302 H412 | -- | -- | -- |

Source: Annex VI Regulation No 1272/2008

Self-classification(s)

Where harmonised classification is not available, suppliers are obliged to decide on the classification of a substance or mixture. This CLP provision is called self-classification.

Self-classifications were retrieved for the seven substances which have an EC number. In the cases where different self-classifications appeared, the classifications most commonly notified are reproduced in Table 1-7, also referring to the total number of notifications for each substance. Notifications made only in a few cases are reproduced in cases where they include stricter classification categories. It should be noted that the fact that a classification is supported by multiple notifications does not necessarily mean that it is correct. There is no conclusive relation between the number of notifications and the correctness of classification, both in cases where the majority support a classification which is more strict and where the opposite is true.

¹³ Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006 (REACH).

Furthermore, experience has lead e.g. DEPA (2010) to the conclusion that the lack of data on hazardous properties of chemicals makes it difficult for companies to meet their obligations to self-classify the chemicals they import or produce. In this sense, though a large number of notifications may be indicative of a large number of users, it cannot be assumed that a lack of notifications is to be concluded as a lack of use of a substance.

Table 1-7: Overview on self-classification

| Substance (CAS) | Classification | | No. of companies notifying this classification |
|---|--|--|--|
| | Hazard Class and Category Code(s) | Hazard statement code(s) | |
| 2,3-Dibromo-1-propanol (CAS 96-13-9) | Acute Tox. 4 Acute Tox. 3 Acute Tox. 4 Carc. 1B Repr. 2 Aquatic Chronic 3 | H302 H311 H332 H350 H361 H412 | 27 out of 27 |
| 1,3-dibromopropan-2-ol (CAS 96-21-9) | Flam. Liq. 3 Acute Tox. 3 Skin Irrit. 2 Eye Irrit. 2 STOT SE 3 Carc. 2 | H226 H301 H315 H319 H335 H351 | 23 out of 27 |
| 1,4-dibromobutan-2-ol (CAS 19398-47-1) | No notifications submitted. | | |
| 1,4-Dibromo-2,3-butanediol (CAS 14396-65-7) | Skin Irrit. 2 Eye Dam. 1 STOT SE 3 | H315 H318 H335 | 23 out of 23 |
| 2,2-bis(bromomethyl)propane-1,3-diol (CAS 3296-90-0) | Acute Tox. 4 Eye Irrit. 2 Muta. 2 | H302 H319 H341 | 355 out of 493 |
| | Eye Irrit. 2 Muta. 1B Carc. 1B STOT RE 2 Aquatic Chronic 4 | H319 H340 H350 H373 H413 | 76 out of 493 |
| | Carc. 2 | H351 | 27 out of 493 |
| | Eye Irrit. 2 | H319 | 24 out of 25 |
| 3-Bromo-2,2-bis(bromomethyl)-1-propanol (CAS 1522-92-5) | Acute Tox. 4 Acute Tox. 4 Skin Irrit. 2 Eye Irrit. 2 Acute Tox. 4 | H302 H312 H315 H319 H332 | 1 out of 25 |
| | Aquatic Chronic 3 | H412 | 69 out of 122 |
| | Aquatic Chronic 3 Eye Irrit. 2 | H412 H319 | 24 out of 122 |
| | Acute Tox. 4 Muta. 2 | H302 H341 | 15 out of 122 |
| | Eye Irrit. 2 Muta. 1B Carc. 1B | H319 H340 H350 | 6 out of 122 |

Source: Compiled from data from: <https://echa.europa.eu/information-on-chemicals/cl-inventory-database>

The self-classification presented above does not point out the carcinogenic potential with a possible mutagenic/genotoxic mode of action of the substances, resulting from the read across performed by DEPA (2016). The results of the read across lead to the proposed grouping of the SBAA, discussed in Section 3.

1.3. Legal status and use restrictions

1.3.1. Regulation of the substance under REACH

The substances described are not subject to **authorization** under REACH.

As for the substance 2,3-dibromopropan-1-ol (CAS 96-13-9), which is harmonized classified as being toxic to reproduction, entry 28 of REACH Annex XVII “**Restrictions** on the Manufacture, Placing on the Market and Use of Certain Dangerous Substances, Mixtures and Articles” applies.

Entry 28 is relevant for substances which appear in Part 3 of Annex VI to Regulation (EC) No 1272/2008, classified as carcinogen category 1A or 1B (Table 3.1) or carcinogen category 1 or 2 (Table 3.2).

According to entry 28, specified substances “*shall not be placed on the market, or used,*

— *as substances,*

— *as constituents of other substances, or,*

— *in mixtures,*

for supply to the general public when the individual concentration in the substance or mixture is equal to or greater than:

— *either the relevant specific concentration limit specified in Part 3 of Annex VI to Regulation (EC) No 1272/2008, or,*

— *the relevant generic concentration limit specified in Part 3 of Annex I of Regulation (EC) No 1272/2008”*

The **registration** obligations applicable under REACH have so far lead to the registration of:

- 2,2-bis(bromomethyl)propane-1,3-diol (CAS 3296-90-0); and
- 2,2-dimethylpropan-1-ol, tribromo derivative (CAS 36483-57-5)

The registration deadline by 31 May 2018 for substances manufactured or imported at 1-100 tonnes a year might result in additional registrations of SBAA, as suggested by the number of self-classifications indicating a use of the substances.

1.3.2. Other legislative measures

The U.S. EPA regulates 2,2-bis(bromomethyl)propane-1,3-diol, (CAS 3296-90-0) under the Toxic Substances Control Act (TSCA). Table 1-8 summarizes the U.S. EPA health and safety data reporting regulations. (NTP 2002)

Table 1-8: U.S. EPA Regulations

| U.S. EPA Regulations | |
|--|---|
| Regulatory action | Effect of regulation and other comments |
| 40 CFR 716 – PART 716 – HEALTH AND SAFETY DATA REPORTING. Promulgated: 51 FR 32726, 09/15/86. U.S. Codes: 15 U.S.C. 2607(d). 2,2-Bis(bromomethyl)-1,3-propanediol has an effective date of 6/1/87 and a sunset date of 12/19/95. | This subpart sets forth requirements for the submission of lists and copies of health and safety studies on chemical substances and mixtures selected for priority consideration for testing rules under section 4(a) of TSCA and on other chemical substances and mixtures for which U.S. EPA requires health and safety information in fulfilling the purposes of TSCA. |

Source: The regulations in this table have been updated through the 1998 Code of Federal Regulations 40 CFR, July 1, 1996; 21 CFR, April 1, 1996; 29 CFR, July 1, 1996.

Source: NTP (2002)

2,2-bis(bromomethyl)propane-1,3-diol (CAS 3296-90-0) is a specified substance in the USEPAs Emergency Planning and Community Right-To-Know Act Toxics Release Inventory. Listed substances are subject to reporting requirements (NTP 2014).

1.3.3. Non-governmental initiatives

Information as to initiatives specifically referring to the use (or to the phase-out) of the substances from the small brominated alkyl alcohol group has not been found. Nonetheless, various initiatives exist in relation to the general use of bromine in EEE, in some cases also prescribing voluntary thresholds for the presence of bromine in EEE articles. This includes among others the following:

- Green labelling schemes: the presence of hazardous substances is sometimes addressed in such schemes through criteria related to the use of various substances. In relation to bromine based substances, the for example, the Blue Angel Label requirements differ from product to product where brominated and chlorinated compounds are concerned. For hair dryers and TV sets, the criterion is that “halogenated polymers shall not be permitted. Neither may halogenated organic compounds be added as flame retardants. Moreover, no flame retardants may be added which are classified pursuant to Table 3.1 or 3.2 in Annex VI to Regulation (EC) 1272/2008 as very toxic to aquatic organisms with long-term adverse effect and labelled with Hazard Statement H 410 or Risk Statement R 50/53.” Process-related, technically unavoidable impurities; fluoroorganic additives used to improve the physical properties of plastics (provided that they do not exceed 0.5 weight percent) and plastic parts less than 25 grams in mass are exempt from this rule (Blue Angel 2012). Nordic Swan requires that organic halogenated flame retardants and other flame retardants assigned one or more of the following risk phrases, or combinations, must not be added: H350, H350i, H340, H360F, H360D, H360Fd, H360Df (Osmani et al. 2014).
- In 2009 iNEMI, the International Electronics Manufacturing Initiative, published a position statement referring to a threshold for the presence of bromine in EEE components specified to be “low halogen”. The position paper supports the following definition of “low halogen” (BFR-/CFR-/PVC-free) electronics: “A component* must meet all of the following requirements to be Low Halogen (“BFR/CFR/PVC-Free”):
 - All printed board (PB) and substrate laminates shall meet Br and Cl requirements for low halogen as defined in IEC 61249-2-21 and IPC-4101B per 1a below (refer to IEC and IPC standards for actual requirements).

- Non-halogenated epoxide with a glass transition temperature of 120°C minimum. The maximum total halogens contained in the resin plus reinforcement matrix is 1500 ppm with a maximum chlorine of 900 ppm and maximum bromine being 900 ppm.
- For components* other than printed board and substrate laminates: Each plastic within the component contains < 1000 ppm (0.1%) of bromine [if the Br source is from BFRs] and < 1000 ppm (0.1%) of chlorine [if the Cl source is from CFRs or PVC or PVC copolymers].”

iNEMI member companies supporting this definition include: Cisco, Dell Inc., Doosan Corporation, HP, Intel Corporation, Lenovo, Nan Ya Plastics Corporation, Senju Comtek Corp. Sun Microsystems, Inc. and Tyco Electronics.

2. Use in electrical and electronic equipment

In relation to applications and uses of the substances of the small brominated alkyl alcohol group, the following research approach has been followed:

- Data was obtained through a search of the substance CAS numbers and where available the substance EC numbers in the following databases:
 - ECHA Information on Chemicals database¹⁴;
 - The Global Portal to Information on Chemical Substances of the OECD eChemPortal¹⁵;
 - TOXNET-Toxicology Data Network - HSDB® (Hazardous Substances Data Bank) of the U.S. National Library of Medicine¹⁶;
 - The National Toxicology Programm, US Department of Health and Human Services; and
 - The SPIN database – Substances in Preparations In the Nordic countries¹⁷.
- Additionally, an internet research with CAS/EC numbers and relevant key words was carried out, identifying among others safety data sheets for some of the substances (most often, the combination of CAS number and the term “material safety data sheet” retrieved such documents).

Detailed information is reproduced below in relation to substances of the SBAA group for which information and data was available.

¹⁴ <http://echa.europa.eu/information-on-chemicals>

¹⁵ <http://www.echemportal.org/echemportal/page.action?pageID=9>

¹⁶ <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

¹⁷ <http://www.spin2000.net>

2.1. 2,3-dibromopropan-1-ol (CAS: 96-13-9), synonym: 2,3-dibromo-1-propanol

2.1.1. Function of the substance

According to the substance profile of the National Toxicology Program of the U.S. Department of Health and Human Services Secretary in its 13th Report on Carcinogens (RoC), 2,3-dibromopropan-1-ol is used as an intermediate in the preparation of flame retardants, insecticides, and pharmaceuticals (NTP 2014a).

A monography on the substance prepared by WHO International Agency for Research on Cancer IARC in the series “Monographs on the Evaluation of Carcinogenic Risks to Humans” (WHO IARC 2000a),¹⁸ specifies the substance to have been used as intermediate in the preparation of flame retardants, insecticides, and pharmaceuticals.

Its main use was in the production of the brominated flame retardant tris(1,2,3-dibromopropyl) phosphate that was used in textiles, commonly called “Tris” (WHO IARC 2000a; NTP 2014a). According to NTP (2014a), the chemical has also been used as a flame retardant as such.

2.1.2. Types of applications / types of materials

According to NTP (2014a), “Tris”, produced from 2,3-dibromopropan-1-ol, was used in the past in the fabrication of children’s clothing and other products, until it was banned from use in sleepwear in 1977 by the Consumer Product Safety Commission after studies showed that it caused cancer in experimental animals.

The IARC monography states that production of this flame retardant other than for research purposes has been discontinued (WHO IARC 2000a). MSDS available on the internet indicate “laboratory chemicals” as recommended use.¹⁹

2.1.3. Quantities of the substance used

2,3-dibromo-1-propanol is not registered under REACH, it is therefore understood either not to be used in the EU or to be applied in low quantities (in which case a volume for the EU could not be concluded in lack of data).

The European Flame Retardant Association, which represents the leading organisations who manufacture, market or use flame retardants in Europe stated in a stakeholder consultation in 2014²⁰ “We do not have any information about 2,3-dibromo-1-propanol, since none of the EFRA member companies manufacture this substance. We thus also believe that its use in E&E should be negligible, if it takes place at all.”

On the other hand, the case of 2,3-dibromo-1-propanol suggests that it is not always clear which (brominated) flame retardant is used within the supply chain. The Test & Measurement Coalition

¹⁸ WHO IARC (2000a): IARC Monographs on the Evaluation of Carcinogenic Risks To Humans, Some Industrial Chemicals Vol. 77; <http://monographs.iarc.fr/ENG/Monographs/vol77/index.php>; substance profile for 2,3-DIBROMOPROPAN-1-OL available at: <https://monographs.iarc.fr/ENG/Monographs/vol77/mono77-17.pdf>

¹⁹ Fisher Scientific safety data sheet at <https://www.fishersci.com/shop/msdsproxy?productName=AC112890050&productDescription=2%2C3-DIBROMOPROPANOL%2C+96%25+5GR2&catNo=AC11289-0050&vendorId=VN00032119&storeId=10652>

²⁰ European Flame Retardants Association EFRA (2014): Contribution submitted during stakeholder consultation on 04.04.2014; http://rohs.exemptions.oeko.info/fileadmin/user_upload/RoHS_Substance_Review/Substance_Profiles/last_contributions/final_EFRA4_answers_to_Oeko-Institute_survey_on_RoHS_04.04.2014__2_.pdf

stated in the above-mentioned stakeholder consultation that an in-depth-survey of the supply chain, including SME custom part suppliers, would be required to determine exposure and whether substitution would impact safety or other qualifications (e.g. for flame-retarded uses such as epoxy internal to power supplies).²¹

The IARC monography states that 2,3-dibromo-1-propanol is only produced for research purposes (WHO IARC 2000a).

In the United States, production of 2,3-dibromo-1-propanol was more than 10 million pounds in 1976, but decreased drastically after the use of “Tris” was banned in sleepwear (NTP 2014a). In 2009, 2,3-dibromo-1-propanol was produced by two manufacturers in East Asia and was available from 16 suppliers, including 9 U.S. suppliers (NTP 2014a). Reports filed in 1986, 1990, and 1998 under the U.S. Environmental Protection Agency’s Toxic Substances Control Act Inventory Update Rule indicated that U.S. production plus imports of 2,3-dibromo-1-propanol totalled 10,000 to 500,000 lb [~ 4,500-225,000 kg]; no inventory update reports for 2,3-dibromo-1-propanol were filed in 1994 or 2002 (NTP 2014a).

2.2. 1,3-dibromopropan-2-ol (CAS: 96-21-9)

2.2.1. Function of the substance

The search for MSDS for 1,3-dibromopropan-2-ol reveals various MSDS available on the internet that indicate uses for research purposes²² / as laboratory chemicals²³ or as certified reference materials²⁴. A MSDS specified by LookChem also indicates uses for research and development.²⁵

2.2.2. Types of applications / types of materials

No data found.

2.2.3. Quantities of the substance used

One supplier, Apollo Scientific Ltd., has been identified in the UK, on the basis of a safety data sheet last updated in October 2015.²⁶ Additional suppliers exist in the UK (Fluorochem) and in the US.

²¹ Test & Measurement Coalition TMC (2014): Contribution submitted during stakeholder consultation on 04.04.2014; http://rohs.exemptions.oeko.info/fileadmin/user_upload/RoHS_Substance_Review/Diisobutylphthalate/20140404_TMC_response_to_Oeko_additional_RoHS_substances__2014-0404.pdf

²² MSDS of Fluorochem Ltd., <https://www.cymitquimica.com/uploads/products/10/pdf/GEG5180-msds.pdf>;
Santa Cruz Biotechnology, Inc.; <http://datasheets.scbt.com/sds/aghs/en/sc-215371.pdf>

²³ MSDS of Fisher Scientific: <https://www.fishersci.ca/viewmsds.do?catNo=AC406541000>

²⁴ MSDS of SPEX CertiPrep Inc.: <http://www.spexcetiprep.com/MSDS/8240-G.pdf>

²⁵ <http://www.lookchem.com/msds/2011-06/9/372404%2896-21-9%29.pdf>

²⁶ MSDS of Apollo Scientific Ltd.; http://www.apolloscientific.co.uk/downloads/msds/OR1061_msds.pdf

2.3. 2,2-bis(bromomethyl)propane-1,3-diol (CAS: 3296-90-0), Synonyms: Dibromoneopentyl-glycol, 2,2-Bis(bromomethyl)-1,3-propanediol

2.3.1. Function of the substance

2,2-bis(bromomethyl)propane-1,3-diol has been used as a flame retardant and as an intermediate (NTP 2014b).

2.3.2. Types of applications / types of materials

According to the ECHA Information on Chemicals database,²⁷ 2,2-bis(bromomethyl)propane-1,3-diol is used in polymers and in the manufacture of plastic products and is also understood to be an intermediate. The substance can be found in plastic based material products such as food packaging and storage, toys and mobile phones according to the ECHA database.

EFSA (2012) lists 2,2-bis(bromomethyl)propane-1,3-diol as a novel BFR: “Novel BFRs are defined as chemicals applied as flame retardants, and with confirmed presence in materials and/or goods in concentrations above 0.1 %” (EFSA 2012).

The SPIN database shows²⁸ that for use categories, Finland registered the use as flame retardants and extinguishing agent in 2013 and the use categories “others” between 2004 to 2008. The SPIN database indicates an article index of 2 or 3, which means that the substance is used in articles.

According to a monography on the substance prepared by WHO International Agency for Research on Cancer IARC in the series “Monographs on the Evaluation of Carcinogenic Risks to Humans” (WHO IARC 2000b),²⁹ 2,2-bis(bromomethyl)propane-1,3-diol is a reactive flame retardant that is used primarily in unsaturated polyester resins for moulded products and in rigid polyurethane foams. This use is also mentioned by Rad et al. (2010).

WHO IARC (2000b) further state that the substance is increasingly used in CFC (chloro-fluorocarbon)-free foam products designed to meet more stringent standards of flame retardancy. Lassen et al. (2014) confirm these applications: “Applications (as indicated by manufacturers) include use in CFC-free foam systems designed to meet more stringent standards of flame retardancy, for example in the product FR-522 produced by ICL” (Lassen et al. 2014).

The research on safety data sheets revealed additional resin products containing the substance, e.g. PolyLite 33441-00 by Reichhold³⁰ and CRYSTIC 356PA by Scott Bader.³¹

According to the substance profile of the National Toxicology Program of the U.S. Department of Health and Human Services Secretary in its 13th Report on Carcinogens (RoC), 2,2-bis(bromomethyl)propane-1,3-diol is also used as a chemical intermediate in the production of pentaerythritol ethers and other derivatives used as flame retardants (NTP 2014b).

²⁷ <https://echa.europa.eu/substance-information/-/substanceinfo/100.019.971>

²⁸ SPIN database, entry for 2,2-bis(bromomethyl)propane-1,3-diol (CAS 3296-90-0): http://195.215.202.234/fmi/xsl/spin/SPIN/maininfo.xsl?-db=SPINstof&-skip=0&-max=1&casnr.op=eq&casnr=3296-90-0&SPINnavn%3a%3anavn.op=eq&SPINnavn%3a%3anavn=&ec_nr.op=eq&ec_nr=&-lay=SPINnavn&-find

²⁹ WHO IARC (2000b): IARC Monographs on the Evaluation of Carcinogenic Risks To Humans, Some Industrial Chemicals Vol. 77; <http://monographs.iarc.fr/ENG/Monographs/vol77/index.php>; substance profile for 2,2-BIS(BROMOMETHYL)PROPANE-1,3-DIOL available at: <https://monographs.iarc.fr/ENG/Monographs/vol77/mono77-18.pdf>

³⁰ MSDS Reichhold, Inc. <https://www.b2bcomposites.com/msds/reichhold/33441-00.pdf>

³¹ MSDS Scott Bader; http://www.flints.co.uk/pdf/crystic_356pa.pdf

Baron et al. (2014) explain that although publically available information on 2,2-bis(bromomethyl)propane-1,3-diol is very scarce, it is understood that low volumes are in use in the EU for the manufacture of plastic articles. Though this could include plastic articles used in EEE, the information provided by stakeholders suggested that this was not the case (see information from ICL-IP Europe in section 2.3.3 below).

In a safety data sheets the following uses have been specified: laboratory chemicals; production of materials.

2.3.3. Quantities of the substance used

2,2-bis(bromomethyl)propane-1,3-diol is registered in the EU for a tonnage band of 100 – 1,000 tonnes per year by the following registrant: ICL-IP Europe B.V. (OR1), Fosfaatweg 48 1013 BM Amsterdam, the Netherlands (ECHA Registered substances database).³²

The registrant stated in a stakeholder consultation in 2014 on "*Compilation and review of quantitative usage information concerning the various substances on the prioritised shortlist*"³³ that "*DBNPG is used solely as a reactive flame retardant in construction, and is used for > 90% in Unsaturated Polyester used for UPE sheets in roofing.*"; ICL-IP further stated that it is not used in EEE (ICL-IP Europe (2014)).

The Test & Measurement Coalition states in relation to this substance that "*Brominated flame retardants not currently restricted under RoHS are still quite pervasive in the supply chain and are frequently noted in supplied article sub-components. As this substance is listed with possible use as a flame retardant for epoxy, polyester, and urethane foams, an in-depth survey of the supply chain, including SME custom part suppliers, would be required to determine exposure and whether substitutions would impact safety or other certifications (e.g. for flame-retarded uses such as epoxy internal to power supplies.)*"

The SPIN database contains data on 2,2-bis(bromomethyl)propane-1,3-diol used in Nordic countries: Data on amounts are confidential, however there are notifications for total use e.g. in 2013 by Denmark, Finland and Norway.

According to the WHO IARC (2000b), information available in 1999 indicated that 2,2-bis(bromomethyl)propane-1,3-diol was manufactured by two companies, one in Israel and one in Ukraine.

US sources state an annual production in the USA of 2,2-bis(bromomethyl)propane-1,3-diol was estimated at over 2,300 kg (5,000 lb) in 1977 and 1979 and at 3 million to 4 million pounds in 1983. 2,2-bis(bromomethyl)propane-1,3-diol was listed by the U.S. Environmental Protection Agency as a high-production-volume chemical in 1990, indicating that annual production exceeded 1 million pounds (NTP 2014b). NTP (2014b) further states that in 2009, 2,2-bis(bromomethyl)propane-1,3-diol was produced by three manufacturers: in the United States; in the Middle East; and in China and was available from 14 suppliers, including 7 U.S. suppliers.

³² ECHA Registered substances database for 2,2-bis(bromomethyl)propane-1,3-diol at <https://echa.europa.eu/registration-dossier/-/registered-dossier/7873>

³³ ICL-IP Europe (2014): Contribution submitted during stakeholder consultation on 02.04.2014; http://rohs.exemptions.oeko.info/fileadmin/user_upload/RoHS_Substance_Review/Substance_Profiles/20140402_ICL_RoHS_OKOinstitute_comments_ICL-IP_Dibromoneopentyl-glycol.pdf

According to EFSA (2012), there are more than 50 suppliers of 2,2-bis(bromomethyl)propane-1,3-diol in the world (EFSA 2012).³⁴

Safety data sheets have been found for suppliers in the UK (Fluorochem and Scott Bader)³⁵, in the US and in China.

2.4. 3-Bromo-2,2-bis(bromomethyl)-1-propanol (CAS 1522-92-5) and 2,2-dimethylpropan-1-ol (CAS: 36483-57-5), tribromo derivative, synonyms: Tribromoneopentyl alcohol

As mentioned above, 3-Bromo-2,2-bis(bromomethyl)-1-propanol (CAS 1522-92-5) and 2,2-dimethylpropan-1-ol (CAS 36483-57-5) have the identical structural formula. Therefore DEPA (2016) considered them as a single substance; as have Lassen et al. (2014). However the substances have different EC numbers and the ECHA Information on Chemicals database lists two different entries. Reports such as e.g. EFSA (2012) refer to only one CAS number. Against this background and for convenience, these substances are referred to together.

2.4.1. Function of the substance

The substance is applied as a reactive intermediate for high molecular weight flame retardants, particularly in the production of phosphorus and bromine containing flame retardants, Lassen et al. (2014) indicate as an example a product named, FR-513 produced by ICL.

2.4.2. Types of applications

According to the ECHA information on chemicals database,³⁶ this substance is used in the manufacture of polymers, plastic products and chemicals and as an intermediate. ECHA has no registered data indicating the type of article into which the substance has been processed.

The SPIN database has data on amounts, which are mostly confidential; the publicly available data indicates the use category "Adhesives, binding agents" and also indicates consumer preparations for 2013, 2012, 2011 and 2010.³⁷ The SPIN database specifies the article index 2 and 3 for 2,2-dimethylpropan-1-ol, meaning that the substance is used in articles.

Safety data sheets available on the internet additionally reveal the following uses:

- The company Polymer Add Pte. Ltd.³⁸ lists as identified uses:
 - It is reactive flame retardant for polyurethanes, where its high solubility in the system makes it especially useful.

³⁴ EFSA (2012): Scientific Opinion on Emerging and Novel Brominated Flame Retardants (BFRs) in Food; EFSA Panel on Contaminants in the Food Chain; EFSA Journal 2012;10(10):2908; <http://onlinelibrary.wiley.com/doi/10.2903/j.efsa.2012.2908/epdf>

³⁵ Fluorochem: [http://www.fluorochem.co.uk/System/DownloadSDS?fileName=\(en-GB\)BR1298_3.00.pdf](http://www.fluorochem.co.uk/System/DownloadSDS?fileName=(en-GB)BR1298_3.00.pdf)
 Scott Bader: <http://www.ecfibreglasssupplies.co.uk/images/SafetyDataSheet/1590.pdf>

³⁶ <https://echa.europa.eu/substance-information/-/substanceinfo/100.048.218>

³⁷ SPIN database, entry for 2,2-dimethylpropan-1-ol (CAS: 36483-57-5); http://195.215.202.234/fmi/xsl/spin/SPIN/spinuset.xml?-db=SPINstof&-skip=0&-max=1&casnr.op=eq&casnr=36483-57-5&SPINnavn%3a%3anavn.op=eq&SPINnavn%3a%3anavn=&ec_nr.op=eq&ec_nr=&-lay=spinuse&-find

³⁸ MSDS Polymer Add Pte; <http://polymeradd.sg/36483-57-5.pdf>

- It is also suitable for use in rigid polyurethane and thermoset polyester resins because of its high bromine content
- It is used alone, as polyol in the formulations of rigid foams.
- The supplier CRC Industries Europe bvba³⁹ provides the PU Foam Fire Resist 2-in-1 Aerosol for sealants and isolation;
- Huntsman Advanced Materials Americas Inc. sells the product RP 6453-1 Resin as a polyurethane resin.⁴⁰
- Fischerwerke GmbH & Co. KG indicates the use of B1-Gun Foam PUFS 750⁴¹ for foaming at constructional elements requiring advanced fire security standards, foaming in thermal insulation composite systems between EPS heat insulation panels, gaps of maximum 70 x 20 mm (depth x width), covered with mineral plaster, ideal construction and insulation foam for filling and sealing of cavities between brick work and window frames, window sills, roller blinds chassis etc., insulating of pipeline mountings.

2.4.3. Quantities of the substance used

The substance is registered for a tonnage band of 100 – 1 000 tonnes per year by the registrant: ICL-IP Europe B.V. (OR1), Fosfaatweg 48 1013 BM Amsterdam The Netherlands Netherlands and for intermediate use only by ICL-IP Terneuzen B.V. (M), Frankrijkweg 6, Havens/Docks 1205-45308 BJ 4538 BJ Terneuzen Netherlands.

EFSA lists 3-Bromo-2,2-bis(bromomethyl)-1-propanol (CAS 1522-92-5) as an emerging BFR: “Emerging BFRs are defined as chemicals which are applied as flame retardants that have been identified as anthropogenic chemicals in any environmental compartment, in wildlife, in food or in humans. The use of the word „emerging“ in this definition does not imply that there is evidence for an increasing trend in the concentration of these BFRs in the environment, in food or in human samples.” According to EFSA (2012), for the substance as many as 79 commercial sources have been indicated.

2.5. General Information for small brominated alkyl alcohols

To summarise the available information, the following uses have been found for the various substances:

2.5.1. Named uses in materials:

- Chemical intermediate for producing pentaerythritol ethers (CAS: 3296-90-0)
- Epoxy (resin) (CAS: 3296-90-0)
- Flame retardant and production of flame retardants (CAS: 96-13-9; CAS: 3296-90-0; CAS 1522-92-5 / 36483-57-5):

³⁹ MSDS CRC Industries Europe bvba; <http://www.farnell.com/datasheets/1714569.pdf>

⁴⁰ MSDS Huntsman Advanced Materials Americas Inc.; <https://www.freemansupply.com/MSDS/Combined/Huntsman/RenPoly/RenPIM6453-1ENG.pdf>

⁴¹ MSDS Fischerwerke GmbH & Co. KG; http://content.fischer.de/cbfiles/Fischer/Zulassungen/ZD_SDB_01_B1_F_%23SDE_%23AIP_%23V1.pdf

- Production of tris(1,2,3-dibromopropyl) phosphate, commonly called TRIS (CAS: 96-13-9)
- Reactive intermediate for production of high molecular weight flame retardants, particularly in the production of phosphorus and bromine containing FRs (CAS: 1522-92-5/36483-57-5)
- Plastics (CAS: 3296-90-0); (CAS: 1522-92-5 / 36483-57-5)
- Polyester (resin) (CAS: 3296-90-0)
- Polymers (CAS: 3296-90-0); (CAS: 1522-92-5 / 36483-57-5)
- Polyol in the formation of rigid foams (CAS: 1522-92-5/36483-57-5)
- Polyurethanes (resin) (CAS: 1522-92-5/36483-57-5)
- Resin products (CAS: 3296-90-0)
- Rigid polyurethane (CAS: 1522-92-5/36483-57-5)
- Rigid polyurethane foam (CAS: 3296-90-0; CAS: 1522-92-5/36483-57-5)
- Thermoset polyester resins (CAS: 1522-92-5/36483-57-5)
- Unsaturated polyester resins (CAS: 3296-90-0) for moulded products
- Urethane foams (CAS: 3296-90-0)
- Production of flame retardants:

2.5.2. Named uses in applications:

- Adhesives, binding agents (CAS 1522-92-5 / 36483-57-5)
- CFC-free foam systems designed to meet more stringent standards of flame retardancy (CAS: 3296-90-0)
- Flame retardants and extinguishing agent (CAS: 3296-90-0; CAS: 96-13-9)
- Foams for construction applications with advanced fire security standards, i.e., insulation, filling, sealing, etc. (CAS: 1522-92-5/36483-57-5)
- Food packaging and storage (CAS: 3296-90-0)
- Intermediate in the production of insecticides (CAS: 96-13-9)
- Intermediate in the production of pharmaceuticals (CAS: 96-13-9)
- Laboratory chemical (96-13-9; CAS: 96-21-9; CAS: 3296-90-0; CAS: 19398-47-1; CAS: 3296-90-0)
- Mobile phones (CAS: 3296-90-0)
- Textiles (children's clothing – past use) (96-13-9)
- Toys (CAS: CAS: 3296-90-0)
- UPE sheets used for roofing (CAS: 3296-90-0)

2.5.3. Information from umbrella specifications for EEE components

Oeko-Institut (2008) explains that the German Electrical and Electronic Manufacturers Association (ZVEI) publishes umbrella specifications of the EEE sector, in which typical components of different electrical and electronic product families are detailed. The Umbrella Specifications aim to comply with the request of customers for detailed material specifications on individual electronic

components, semiconductors, passive components, printed circuit boards, and electromechanical components. Furthermore, the Umbrella Specifications were developed against the background of the International Material Data System (IMDS) introduced by the automotive industry. While the IMDS requires material contents data in IMDS format for each individual component, the Umbrella Specifications are based on the presentation of special product families with typical characteristics whereby the number of varying inputs will be drastically reduced. The Umbrella Specifications have been elaborated jointly by a number of electronic component manufacturers. From a screening of the current Umbrella specifications published by ZVEI⁴², it has been identified that resins of relevance to SBAA are applied in certain component groups. These are specified in Table 2-1 along with relevant information reproduced from the specifications.

⁴² See: <http://www.zvei.org/Verband/Fachverbaende/ElectronicComponentsandSystems/Seiten/Umbrella-Specifications.aspx>

Table 2-1: Use of resins in EEE components, as specified in umbrella specifications published by ZVEI

| Title | Product class | Product part (IMDS: semi component) | Material (IMDS Material) | Material (Classification) ISO 22628 / VDA 231 | Substance | typical mass of substance [wt%] | CAS if applicable (of material) | typical mass of material [wt-%] | Source (file name and specified date) |
|--|------------------------------|-------------------------------------|--------------------------|---|----------------------------|---------------------------------|---------------------------------|---------------------------------|--|
| Metallised Film Capacitor for EMI Suppression Class X2 | Metallised Polypropylene | Encapsulation | Polymer | 2C | PU/Epoxy | 24,8 | | 58,5 | EMI Suppression Class X2 Ts; 29.10.2009 |
| | | | Hydroxide | | Al(OH)3 | 37,2 | 21645-51-2 | | |
| | | | Polymer | 2A | PBT | 34,2 | | | |
| | | | Oxide | | SB2O3 | 1,9 | 1309-64-4 | | |
| | | | Flame retardant | | Equivalent Br | 1,9 | | | |
| Metallized Film Capacitor | Film Chip Capacitor ECHU (X) | Active part | Polymer | 2A | Thermosetting resin | 100 | | 40,9 | U_Specs_Film_ECHU_X-IMDS_; Dec 09 |
| | | Termination | Polymer | 2C | Phenolic resin | 7,98 | 9003-35-4 | 12,3 | |
| Metallized Film Capacitor | Film Chip Capacitor ECPU (A) | Termination | Polymer | 2C | Phenolic resin | 7,98 | 9003-35-4 | 13,4 | U_Specs_Film_ECPU_A__IMDS; Dec 09 |
| Metallized Film Capacitor | Film Chip Capacitor ECWU (X) | Termination | Polymer | 2C | Phenolic resin | 7,98 | 9003-35-4 | 13,4 | U_Specs_Film_ECWU_X_-IMDS; Dec 09 |
| NTC | Leaded Disks | Encapsulation | Organic Polymer | 5B | Lacquer [1] or | 100 | | 4 | U_Specs_NTC Leaded Disks K_S; 01.08.2009 |
| | | | | 2C | Epoxy Resin [2] | | | | |
| NTC | Leaded Disks | Encapsulation | Organic Polymer | 5B | Lacquer [1] or | 100 | | 4 | U_Specs_NTC Leaded Disks K_S_neu; 01.08.2009 |
| | | | | 2C | Epoxy Resin [2] | | | | |
| NTC | Leaded Disks | Encapsulation | Organic Polymer | 5B | Lacquer [1] or | 100 | | 4 | U_Specs_NTC Leaded Disks M_S; 01.08.2009 |
| | | | | 2C | Epoxy Resin [2] | | | | |
| NTC | Leaded Disks | Encapsulation | Organic Polymer | 5B | Lacquer [1] or | 100 | | 4 | U_Specs_NTC Leaded Disks M_S_neu; 01.08.2009 |
| | | | | 2C | Epoxy Resin [2] | | | | |
| NTC | Leaded Disks | Encapsulation | Organic Polymer | 2C | Epoxy Resin | 100 | 25928-94-3 | 20 | U_Specs_NTC Leaded Disks S871_S875_S881_S885; 01.08.2009 |

| Title | Product class | Product part (IMDS: semi component) | Material (IMDS Material) | Material (Classification) ISO 22628 / VDA 231 | Substance | typical mass of substance [wt%] | CAS if applicable (of material) | typical mass of material [wt-%] | Source (file name and specified date) |
|---------------------------------|------------------------------------|---|--------------------------|---|---|---------------------------------|---------------------------------|---------------------------------|---|
| NTC | Miniature Sensor insulated leads | Leads | Organic Polymer | 2A | PTFE / other thermoplastic polymer | 100 | | 33 | U_Specs_NTC Miniatur Sensor insulated leads; 01.08.2009 |
| | | Encapsulation | Organic Polymer | 2C | Epoxy Resin | 100 | 25928-94-3 | 17 | |
| NTC | Miniature Sensor uninsulated leads | Encapsulation | Organic Polymer | 2C | Epoxy Resin | 100 | 25928-94-3 | 28 | U_Specs_NTC Miniatur Sensor uninsulated leads; 01.08.2009 |
| Inductive components class A -Ω | S22 | Active Part | Metal (wire) | 1C | Cu | 99,20% | 7440-50-8 | 40 | USpec_Inductors_231110a; 2010 10 16 |
| | | | | | PUR etc. | 0,80% | | | |
| | | Plastic | Duroplaste | 2C ISO 1043 | EP, PA, PUR , PET , PBT , Silicone, etc. | 60 | - | 35 | |
| | | (Insulation, Encapsulation and Potting) | | | Fibre glass, Flame retardant , Additive | 40 | | | |
| Varistor | Disk Varistor | Encapsulation | Organic Polymer | 2C | SiO2 | 49 | 60676-86-0 | 16 | U_Specs_Varistor Disk; 01.08.2009 |
| | | | | | Epoxy Resin | 35 | 25068-38-6 | | |
| | | | | | Brominated epoxy | 12 | 68929-70-1 | | |
| | | | | | Sb2O3 | 2,5 | 1309-64-4 | | |
| | | | | | Additives*) | 1,5 | | | |
| PTC | Switching Applications | Encapsulation | Organic Polymer | 2A | PBT GF(30) FR(17) | 100 | 26062-94-2 | 62 | U_Specs_PTC Switching Applications; 01.08.2009 |

Source: <http://www.zvei.org/Verband/Fachverbaende/ElectronicComponentsandSystems/Seiten/Umbrella-Specifications.aspx>

2.6. Summary of information on uses of small brominated alkyl alcohols

From the available information it seems that there are two main areas of application that could be relevant for the SBAA group in EEE.

The first regards the use of these substances in various types of resins. In light of the molecular structure and in some cases lower melting and boiling points, it is understood that the characteristics of some of the substances in this group would be suitable for use as constituents of various types of resins. This is also supported in some cases by general information related to the use in such materials, for example in epoxy resins, in polyurethane resins, in polyester resins and in resin products in general. There is also information showing that resins are used among others in sub-components of EEE, applied for sealing and encapsulating purposes and in some cases understood to be quite common, such as in components for which umbrella specifications exist.

In parallel it is possible that certain substances in the SBAA group are used in the production of plastics. Though such uses may be less common for substances with lower melting and boiling points, which are likely to vaporise during processing, it is observed that a few of the substances have a melting point around 100°C and a boiling point above 300°C and may thus be used in the production of plastic materials.

3. Human health hazard profile

The following human health hazard profile is based on the information and conclusions regarding the critical endpoints for small linear and branched brominated alkyl alcohols, including 2,2-bis(bromomethyl)-1,3-propanediol (CAS: 32-96-0), 2,3-dibromo-1-propanol / 1,3-dibromo-2-propanol (CAS 96-13-9 / 96-21-9), and 2,2-bis-(bromomethyl)-3-bromo-1-propanol (CAS: 36483-57-5 / 1522-92-5) provided in the report from DEPA (2016) prepared by Wedebye *et al.*, DTU Food.

In the data search for the DEPA report relevant experimental data on human health effects were found for the above mentioned three category members. In addition, information regarding existing guidance values in the form of derived no effect levels or derived minimal effect levels (DNELs/DMELs) and occupational exposure levels have been searched in the publicly available REACH registration dossiers and in the open literature. With regard to information from the REACH registration dossiers, it should be stressed that information provided by registrants has not been subject to scrutiny by ECHA or any EU expert group, or by the authors of this report. However, no DMEL values derived based on non-threshold effects were identified in the available dossiers or in the publicly available literature.

3.1. 2,2-bis(bromomethyl)propane-1,3-diol (CAS: 3296-90-0)

3.1.1. Critical endpoint

In the report from DEPA (2016) prepared by Wedebye *et al.*, experimental data on human health effects was collected and the critical effect for the substance was determined based on these data.

The critical effect for 2,2-bis(bromomethyl)-1,3-propanediol is considered to be the multi-site, multispecies carcinogenic effect, most probably caused by a direct genotoxic action of the parent compound.

This conclusion is based on data from a two-year study with administration of a substance containing 78.6% 2,2-bis(bromomethyl)-1,3-propanediol in the diet to rats and mice. Here, significantly dose-related increases in the incidences of neoplasms were obtained at numerous sites in male and female rats, and to a lesser extent in mice (DEPA 2016).

Suggested classifications of DBNPG specified in industry notifications include classification as mutagenic and carcinogenic: Muta 1B H440/Muta 2 H341 and Carc. 1B H350/ Carc. 2 H351.

3.1.2. Existing Guidance values (DNELs, OELs)

No existing guidance values from official authorities have been identified. The following guidance values have been submitted by the industry as part of the REACH registration dossier. These values are not verified by official authorities.

Table 3-1: Guidance values for 2,2-bis(bromomethyl)propane-1,3-diol (CAS: 3296-90-0)

| Population | Description | Local / systemic effect | Exposure duration | Value | Most sensitive endpoint | Reference |
|------------|-------------------------|-------------------------|--------------------|--|-------------------------|--|
| Workers | Hazard via dermal route | Systemic | Acute / short term | DNEL: 100 mg/kg bw/day (AF=100) | Acute toxicity | REACH registration dossier (ECHA 2016) |
| | | Local | Acute / short term | DNEL: 1.4 mg/cm ² (AF = 20) | Acute toxicity | REACH registration dossier (ECHA 2016) |

AF = Assessment factor

3.2. 2,3-dibromopropan-1-ol (CAS: 96-13-9) and 1,3-dibromopropan-2-ol (CAS: 96-21-9)

3.2.1. Critical endpoint

In the report from DEPA (2016) experimental data on human health effects was collected and the critical effect for the substance was determined based on these data.

The critical effect for 2,3-dibromopropan-1-ol is considered to be the multi-site, multispecies carcinogenic effect, most probably caused by a genotoxic metabolite of the parent compound.

This conclusion is based on data from a two-year study with dermal exposure of rats and mice to 2,3-dibromopropan-1-ol. Here, significantly dose-related increases in the incidences of neoplasms were obtained at numerous sites in male and female rats, and to a lesser extent in mice (DEPA, 2016).

The harmonised classification of 2,3-dibromopropan-1-ol include classification as carcinogenic: Carc. 1B H350.

3.2.2. Existing Guidance values (DNELs, OELs)

This substance is only pre-registered and no existing guidance values have been identified.

3.3. 2,2-dimethylpropan-1-ol, tribromo derivative (CAS: 36483-57-5 and 1522-92-5)

3.3.1. Critical endpoint

In the report from DEPA (2016), experimental data on human health effects were collected and the critical effect for the substance was determined based on these data.

The critical effect for 2,2-dimethylpropan-1-ol, tribromo derivative is considered to be a possible carcinogenic effect, most probably caused by a genotoxic metabolite of the parent compound.

This conclusion is based on data from two repeated dose studies of 14 and 30 days duration, respectively. In the 30-day study renal tubular damage was observed in the kidney and generalized hyperplasia in the urinary bladder. The substance, 2,2-dimethylpropan-1-ol, tribromo derivative, has furthermore shown mutagenic/genotoxic activity *in vitro* in the presence of a metabolic activation system. (DEPA, 2016).

Suggested classifications of the substance specified in industry notifications include classification as mutagenic and carcinogenic: Muta 1B H440/Muta 2 H341 and Carc. 1B H350.

3.3.2. Existing Guidance values (DNELs, OELs)

No existing guidance values from official authorities have been identified. The following guidance values have been submitted by the industry as part of the REACH registration dossier. These values are not verified by official authorities.

Table 3-2: Existing guidance values for 2,2-dimethylpropan-1-ol, tribromo derivative; TBNPA (CAS: 36483-57-5 and 1522-92-5)

| Population | Description | Local / systemic effect | Exposure duration | Value | Most sensitive endpoint | Reference |
|------------|-----------------------------|-------------------------|--------------------------------|---|-------------------------|--|
| Workers | Hazard via inhalation route | Systemic | Long term | DNEL: 2.94 mg/m ³ (AF = 150) | Repeated dose toxicity | REACH registration dossier (ECHA 2016) |
| | | | Acute / short term | Low hazard (no threshold derived) | | REACH registration dossier (ECHA 2016) |
| | | Local | Acute / short term / long term | No hazard identified | | REACH registration dossier (ECHA 2016) |
| | Hazard via dermal route | Systemic | Long term | DNEL: 0.83 mg/kg bw/day (AF = 600) | Repeated dose toxicity | REACH registration dossier (ECHA 2016) |
| | | | Acute / short term | Low hazard (no threshold derived) | | REACH registration dossier (ECHA 2016) |
| | | Local | Acute / short term / long term | No hazard identified | | REACH registration dossier (ECHA 2016) |

| Population | Description | Local / systemic effect | Exposure duration | Value | Most sensitive endpoint | Reference |
|--------------------|-----------------------------|-------------------------|--------------------------------|---|-------------------------|--|
| | Hazard for the eyes | Local | | Medium hazard (no threshold derived) | | REACH registration dossier (ECHA 2016) |
| General population | Hazard via inhalation route | Systemic | Long term | DNEL: 0.72 mg/m ³ (AF = 300) | Repeated dose toxicity | REACH registration dossier (ECHA 2016) |
| | | | Acute / short term | Low hazard (no threshold derived) | | REACH registration dossier (ECHA 2016) |
| | | Local | Acute / short term / long term | No hazard identified | | REACH registration dossier (ECHA 2016) |
| | Hazard via dermal route | Systemic | Long term | DNEL: 0.42 mg/kg bw/day (AF = 1200) | Repeated dose toxicity | REACH registration dossier (ECHA 2016) |
| | | | Acute / short term | Low hazard (no threshold derived) | | REACH registration dossier (ECHA 2016) |
| | | Local | Acute / short term / long term | No hazard identified | | REACH registration dossier (ECHA 2016) |
| | Hazard via oral route | Systemic | Long term | DNEL: 0.42 mg/kg bw/day (AF = 1200) | Repeated dose toxicity | REACH registration dossier (ECHA 2016) |
| | | | Acute / short term | Low hazard (no threshold derived) | | REACH registration dossier (ECHA 2016) |
| | Hazard for the eyes | Local | | Medium hazard (no threshold derived) | | REACH registration dossier (ECHA 2016) |

3.3.3. Summary on health hazards

In the report from DEPA (2016) experimental data on human health effects for the three category members have been reviewed. Based on these data the critical effect of the substances was identified as a multiple-organ carcinogenic effect, most probably exerted by a genotoxic mode of action either by the parent compound itself (2,3-dibromo-1-propanol) or by a metabolite of the parent compound (DEPA, 2016).

One category member, 2,3-dibromo-1-propanol, has a harmonised classification as carcinogenic in category 1B (Carc 1B). Some industry self-classifications include a similar classification as Carc. 1B and also Muta. 1B for 2,2-bis(bromomethyl)-1,3-propanediol, and for the 2,2-dimethylpropan-1-ol, tribromo derivative, industry has suggested classifications as mutagenic in category 2 (Muta. 2). Based on read-across justified by results of experimental data, QSAR predictions for the carcinogenic and mutagenic/genotoxic properties and the harmonised and notified classifications, the classification as carcinogenic in category 1B (Carc. 1B) should be considered for all category members.

4. Environmental hazard profile

The following environmental hazard profiles are based on a data/literature search primarily via OECD's eChem Portal, ECHA's REACH registration data, US EPA's ECOTOX database and the

Danish (Q)SAR database complemented with a general Internet search for public available literature on the selected substances. All identified data, i.e. both experimental and predicted (QSAR) data is presented in the tables.

For two of the substances, the profile is to a certain extent based on REACH registration dossiers data available on ECHA's website. It should be noted that only limited information is presented in the publicly available summaries of the confidential substance registration reports. Furthermore, the information provided by the registrant has not been subject to scrutiny by ECHA or any EU expert group, or by the authors of this report.

4.1. 2,2-bis(bromomethyl)propane-1,3-diol (CAS: 3296-90-0)

4.1.1. Environmental fate

Table 4-1: Data for 2,2-bis(bromomethyl)propane-1,3-diol (CAS: 3296-90-0)

| Property | Endpoint | Value | Reference |
|---|---------------------------|--|--|
| Abiotic degradation, Hydrolysis | T _{1/2} | > 1 year (pH 4 and 7), approx. 1 year (pH 9) at 25°C | REACH registration dossier (ECHA 2016) |
| Biodegradation in water (screening tests) | CO ₂ evolution | 25 % (28d) Not readily biodegradable | REACH registration dossier (ECHA 2016) |
| | DOC removal | 44% degradation (33 d) Inherently biodegradable | REACH registration dossier (ECHA 2016) |
| | BOD | 3 – 33 % (28d) | Statens forurens-ningstilsyn (2008) |
| Bioaccumulation | BCF | <4.8 L/kg | REACH registration dossier (ECHA 2016) |
| | | 2.3 L/kg | Danish (Q)SAR Database |
| Sorption (soil) | Log K _{oc} | < 1.25 | REACH registration dossier (ECHA 2016) |
| | | 0.69 | Danish (Q)SAR Database |
| | | 1.6 | EFSA (2012) |
| Distribution coefficient (octanol/water) | Log K _{ow} | 0.41 | EFSA (2012) |
| | | 1.06 | Danish (Q)SAR Database |
| Atmospheric oxidation (OH) | T _{1/2} | 1.2 days | Danish (Q)SAR Database |

4.1.2. Environmental effects

Table 4-2: Data for 2,2-bis(bromomethyl)propane-1,3-diol (CAS: 3296-90-0)

| Compartment | Organism Species | Type of test | Endpoint | Value | Reference |
|-------------|-----------------------------|-----------------------|------------------|---------|--|
| Water | Algae <i>Desmodesmus</i> | (Short term) (72h) | EC ₅₀ | 37 mg/L | REACH registration dossier (ECHA 2016) |

| Compartment | Organism Species | Type of test | Endpoint | Value | Reference |
|-------------|---|---------------|------------------|-------------------|--|
| | <i>subspicatus</i> (formerly known as <i>Scenedesmus subspicatus</i>) | | NOEC | 12.5 mg/L | REACH registration dossier (ECHA 2016) |
| | Algae <i>Pseudokirchneriella subcapitata</i> (formerly known as <i>Selenastrum capricornutum</i>) | (Acute) (72h) | EC ₅₀ | 97 mg/L | Danish (Q)SAR Database |
| | Daphnia <i>Daphnia magna</i> | Acute (48h) | EC ₅₀ | > 100 mg/L | REACH registration dossier (ECHA 2016) |
| | | | NOEC | 56 mg/L | REACH registration dossier (ECHA 2016) |
| | | | EC ₅₀ | 301.9 | Danish (Q)SAR Database |
| | Fish <i>Onchorhynchus mykiss</i> | Acute (96h) | LC ₅₀ | > 100 mg/L | REACH registration dossier (ECHA 2016) |
| | Fish <i>Pimephales promelas</i> | Acute (96h) | LC ₅₀ | > 447.5 mg/L | Danish (Q)SAR Database |
| STP | Activated sludge (Microorganisms) | Acute (3h) | EC ₅₀ | 320 mg/L | REACH registration dossier (ECHA 2016) |
| Soil | Earthworm <i>Eisenia foetida</i> | Acute (14d) | LC ₅₀ | 540 mg/kg soil dw | REACH registration dossier (ECHA 2016) |
| | | | NOEC | 180 mg/kg soil dw | REACH registration dossier (ECHA 2016) |

4.1.3. Existing guidance values (PNECs)

No existing guidance values from official authorities have been identified. The following guidance values have been submitted by the REACH registrant and have not been verified or approved by official authorities.

Table 4-3: Data for 2,2-bis(bromomethyl)propane-1,3-diol (CAS: 3296-90-0)

| Organisms | Compartment | PNEC value | Reference |
|-----------------------|------------------------|-----------------|--|
| Aquatic organisms | Freshwater | 0.037 mg/L | REACH registration dossier (ECHA 2016) |
| | Marine water | 0.004 mg/L | REACH registration dossier (ECHA 2016) |
| | Intermittent releases | 0.37 mg/L | REACH registration dossier (ECHA 2016) |
| | STP | 21 mg/L | REACH registration dossier (ECHA 2016) |
| | Sediment, freshwater | 0.037 mg/ kg dw | REACH registration dossier (ECHA 2016) |
| | Sediment, marine water | 0.004 mg/kg dw | REACH registration dossier (ECHA 2016) |
| Terrestrial organisms | Soil | 0.54 mg/kg dw | REACH registration dossier (ECHA 2016) |

4.1.4. PBT and vPvB assessment

Persistence (P)

Laboratory experiments show that abiotic degradation of the substance via hydrolysis is ≥ 1 year and data from the REACH dossier show that 2,2-bis(bromomethyl)propane-1,3-diol is not readily biodegradable (25% degr., 28d) but can probably be considered inherently biodegradable (44% degr., 33d). According to the available data and the PBT screening criteria reported in ECHA Guideline on PBT assessment⁴³, 2,2-bis(bromomethyl)propane-1,3-diol does fulfil the screening criteria for P (not ready biodegradable and inherently biodegradability is $< 70\%$) and is therefore potentially P or vP.

This is supported by data from the Canadian domestic substance list, where the substance is categorized as persistent (Canadian DSL, n.d.)

Bioaccumulation (B)

The BCF of the substance is < 2000 L/kg and the substance does not meet the REACH Annex XIII criteria for either B or vB.

Toxicity (T)

Data are available for the acute toxicity of 2,2-bis(bromomethyl)propane-1,3-diol to fish, aquatic invertebrates and algae, where the lowest $L(E)C_{50}$ is 97 mg/L determined over 72 hours for algae. Data for chronic toxicity is also available for algae (the most sensitive species in acute/short term tests), where the 72 h-NOEC for algae is 12.5 mg/L. However, the substance has a notified classification of Carc 1B (see section 3.1.1) for human toxicity (notified by the registrant) and thus the substance may fulfil the REACH Annex XIII criteria for T.

Conclusion on assessment

The available data suggests that the substance does not meet the REACH Annex XIII criteria for B and vB, but possibly for T, P and vP.

4.2. 2,3-dibromopropan-1-ol (CAS: 96-13-9) and 1,3-dibromopropan-2-ol (CAS: 96-21-9)

4.2.1. Environmental fate

Table 4-4: Data for 2,3-dibromopropan-1-ol (CAS: 96-13-9) and 1,3-dibromopropan-2-ol (CAS: 96-21-9)

| Property | Endpoint | Value | Reference |
|---|-----------|-------------------|---------------------------|
| Abiotic degradation, Hydrolysis | $T_{1/2}$ | No available data | |
| Biodegradation in water (screening tests) | | No available data | |
| Bioaccumulation | BCF | 3 | HSDB (based on modelling) |
| | | 3.2 | Danish (Q)SAR Database |

⁴³ https://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf, page 37

| Property | Endpoint | Value | Reference |
|--|---------------------|----------|---------------------------------|
| Sorption (soil) | K _{oc} | 4 | HSDB (based on modelling) |
| | | 11.08 | Danish (Q)SAR Database |
| Distribution coefficient (octanol/water) | Log K _{ow} | 0.96 | HSDB and Danish (Q)SAR database |
| Atmospheric oxidation | T _{1/2} | 8 days | HSDB (based on modelling) |
| | | 5.2 days | Danish (Q)SAR Database |

4.2.2. Environmental effects

Table 4-5: Data for 2,3-dibromopropan-1-ol (CAS: 96-13-9) and 1,3-dibromopropan-2-ol (CAS: 96-21-9)

| Compartment | Organism Species | Type of test | Endpoint | Value | Reference |
|-------------|---|-------------------|------------------|--------------|-----------------|
| Water | Algae <i>Desmodesmus subspicatus</i> (formerly known as <i>Scenedesmus subspicatus</i>) | Acute (48-96h) | EC ₅₀ | 280-550 mg/L | ECOTOX database |
| | Daphnia <i>Daphnia magna</i> | Acute (24-48h) | EC ₅₀ | 185-703 mg/L | ECOTOX database |
| | | Chronic (21d) | NOEC | 9.6-16 mg/L | ECOTOX database |
| | Fish <i>Pimephales promelas</i> | Acute (96h) | LC ₅₀ | 71 mg/L | ECOTOX database |
| STP | Activated sludge (Microorganisms) | No available data | | | |
| Soil | No available data | | | | |

4.2.3. Existing guidance values (PNECs)

No existing guidance values have been identified for 2,3-dibromopropan-1-ol (CAS: 96-13-9) and 1,3-dibromopropan-2-ol (CAS: 96-21-9).

4.2.4. PBT and vPvB assessment

Persistence (P)

There are no available data on the biotic and abiotic degradation of the substance, and it can therefore not be assessed if the substance meets the REACH Annex XIII criteria for a persistent or very persistent substance.

QSAR data for 2,3-dibromopropan-1-ol (CAS no. 96-13-9) suggest that the substance is not readily biodegradable, but the QSAR predictions are outside applicability domain and should therefore only be used as very indicative (Danish (Q)SAR database, n.d).

Bioaccumulation (B)

Data for the log K_{ow} (< 3) as well as the BCF ($<< 2000$ L/kg) show a low potential for bioaccumulation and REACH Annex XIII criteria for both B and vB are not fulfilled for the substance.

Toxicity (T)

Data are available for the acute toxicity of the substance to fish, aquatic invertebrates and algae, where the lowest L(E)C₅₀ is 71 mg/L determined over 96h for fish. There are no data for chronic toxicity available for fish. A 21d chronic test with *Daphnia magna* resulted in a NOEC of 9.6 mg/L as the lowest. However, the substance has a harmonised classification of Carc 1B (see section 3.2.1) and thus the substance fulfils the REACH Annex XIII criteria for T.

Conclusion on assessment:

The substance fulfils the REACH Annex XIII criteria for T. The available data suggests that the substance does not meet the REACH Annex XIII criteria for B and vB. It is not considered possible to conclude on the possible fulfilment of the P or vP criteria for the substance based on the available data.

4.3. 2,2-dimethylpropan-1-ol, tribromo derivative (CAS: 36483-57-5 and 1522-92-5)

4.3.1. Environmental fate

Table 4-6: Data for 2,2-dimethylpropan-1-ol, tribromo derivative (CAS: 36483-57-5 and 1522-92-5)

| Property | Endpoint | Value | Reference |
|---|---------------------------|---|--|
| Abiotic degradation, Hydrolysis | T _{1/2} | > 1 year (pH 4 and pH7) at 50°C 7.5 years (pH 9) at 25°C | REACH registration dossier (ECHA 2016) |
| Biodegradation in water (screening tests) | DOC removal | 77% degradation (36d) "Readily biodegradable" | REACH registration dossier (ECHA 2016) |
| | CO ₂ evolution | 2.5% degradation (28d) "not readily biodegradable" | REACH registration dossier (ECHA 2016) |
| | | Not ready biodegradable ² | Danish (Q)SAR Database |
| | | The compound has a relatively strong resistance to biodegradation and therefore classified as not readily biodegradable (0-7% degradation after 28 days) ¹ . | EFSA (2012) |
| Bioaccumulation | BCF | 14.21 L/kg | REACH registration dossier (ECHA 2016) (QSAR data) |
| Sorption (soil) | K _{oc} | 57.31 L/kg | REACH registration dossier (ECHA 2016) (QSAR data) |
| | | 315 ¹ | EFSA (2012) |
| Distribution coefficient (octanol/water) | Log K _{ow} | 2.25 | Danish (Q)SAR Database |
| | | 2.06 ¹ | EFSA (2012) |
| Atmospheric oxidation (OH) | T _{1/2} | 2.1 days | Danish (Q)SAR Database |

¹ Data for CAS no. 1522-92-5 / ² Conclusion for both CAS no. 36483-57-5 and 1522-92-5

4.3.2. Environmental effects

Table 4-7: Data for 2,2-dimethylpropan-1-ol, tribromo derivative (CAS: 36483-57-5 and 1522-92-5)

| Compartment | Organism Species | Type of test | Endpoint | Value | Reference |
|-------------|---|----------------|------------------|--------------|--|
| Water | Algae <i>Pseudokirchneriella subcapitata</i> (formerly known as <i>Selenastrum capricornutum</i>) | (Acute) (72h) | EC ₅₀ | 28 mg/L | REACH registration dossier (ECHA 2016) |
| | | | NOEC | 2.2 mg/L | REACH registration dossier (ECHA 2016) |
| | Daphnia <i>Daphnia magna</i> | Acute (48h) | EC ₅₀ | 64 mg/L | REACH registration dossier (ECHA 2016) |
| | | | NOEC | 32 mg/L | REACH registration dossier (ECHA 2016) |
| | Fish <i>Cyprinus carpio</i> | Acute (96h) | LC ₅₀ | 32 mg/L | REACH registration dossier (ECHA 2016) |
| | Fish <i>Cyprinus carpio</i> | Chronic (14d) | NOEC | 5.6 mg/L | REACH registration dossier (ECHA 2016) |
| STP | Activated sludge (Microorganisms) | Acute (30 min) | EC ₅₀ | Ca. 400 mg/L | REACH registration dossier (ECHA 2016) |
| | | | EC ₂₀ | Ca. 20 mg/L | REACH registration dossier (ECHA 2016) |
| Soil | No data | | | | |

4.3.3. Existing guidance values (PNECs)

No existing guidance values from official authorities have been identified. Following guidance values have been submitted by the industry and have not been verified by official authorities.

Table 4-8: Data for 2,2-dimethylpropan-1-ol, tribromo derivative (CAS: 36483-57-5 and 1522-92-5)

| Organisms | Compartment | PNEC value | Reference |
|-----------------------|------------------------|----------------|--|
| Aquatic organisms | Freshwater | 0.044 mg/L | REACH registration dossier (ECHA 2016) |
| | Marine water | 0.004 mg/L | REACH registration dossier (ECHA 2016) |
| | Intermittent releases | 0.28 mg/L | REACH registration dossier (ECHA 2016) |
| | STP | 4 mg/L | REACH registration dossier (ECHA 2016) |
| | Sediment, freshwater | 1.19 mg/kg dw | REACH registration dossier (ECHA 2016) |
| | Sediment, marine water | 0.119 mg/kg dw | REACH registration dossier (ECHA 2016) |
| Terrestrial organisms | Soil | 0.046 mg/kg dw | REACH registration dossier (ECHA 2016) |
| Predators | Secondary poisoning | 1 mg/kg food | REACH registration dossier (ECHA 2016) |

4.3.4. PBT and vPvB assessment

Persistence

There are no data available regarding the half-life of substance, and it is therefore not possible to assess whether the substance meets the REACH Annex XIII persistence (P) or very persistent (vP) criteria.

Different data regarding the biodegradability study are available. An inherent biodegradability study (OECD guideline 302B) shows a decrease in DOC concentration of 77% during a period of 36 days (from the REACH registration dossier for CAS no. 36483-57-5 (ECHA, 2016)), where results from a ready biodegradability test show that the substance is not readily biodegradable (2.5%, 28d). Other data also suggest that the substance is not readily biodegradable (QSAR data and data cited in EFSA (2012)). In a report by Statens forurensningstilsyn (2008) (the Norwegian EPA) two studies are cited, where the half-life of TNBPA is estimated to be approximately 100 year, which according to the authors suggests that TNBPA is persistent in the aquatic environment. In summary, by weight of evidence the result of the DOC-based degradation study is considered to be not reliable and is therefore not used in the PBT assessment.

Based on above data and considerations and the PBT screening criteria reported in ECHA Guideline on PBT assessment⁴⁴, it is assessed as likely that the substance fulfils the screening criteria for P (<60% biodegradation ThOD, CO₂ evolution) and is therefore potentially P or vP.

Bioaccumulation

The BCF of the substance is <<2000 L/kg and the substance does not meet the criteria for either B or vB.

Toxicity

Data are available for the acute toxicity of substance to fish, aquatic invertebrates and algae, where the lowest L(E)C₅₀ is 28 mg/L determined over 72 hours for algae. Data for chronic toxicity is also available for algae (the most sensitive species), where the 72 h-NOEC for algae is 2.2 mg/L. However, the substance has a notified classification of Carc 1B (see section 3.3.1) for human toxicity (notified by the REACH registrants) and thus the substance may fulfil the REACH Annex XIII criteria for T.

Conclusion on assessment

The available data suggests that the substance does not meet the REACH Annex XIII criteria for B but possibly for P and T. The substance is not considered a vP or vB substance based on available data.

4.3.5. Summary on environmental hazards

Based on the available data, 2,2-bis(bromomethyl)propane-1,3-diol and 2,2-dimethylpropan-1-ol, tribromo derivative are both considered potentially persistent or very persistent in the environment. It is not possible to make a conclusion on the potential for persistency for 2,3-dibromopropan-1-ol. None of the three substances are assumed to be bioaccumulative in the environment. The ecotoxicity of all three substances towards aquatic organisms representing three different trophic

⁴⁴ https://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf, page 37

levels (fish, invertebrates and algae) is found to be low. However, due to carcinogenic and mutagenic/genotoxic effects towards humans, all three substances are considered to fulfil the REACH Annex XIII criteria for toxicity.

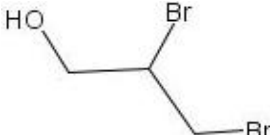
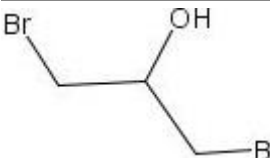
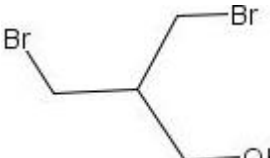
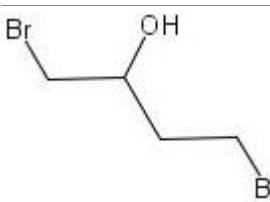
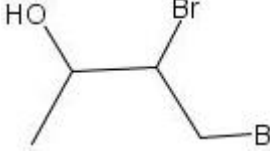
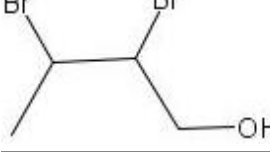
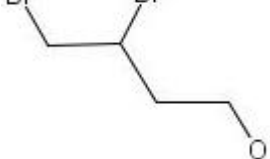
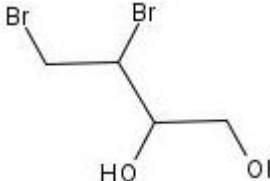
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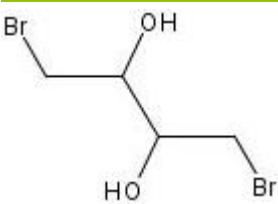
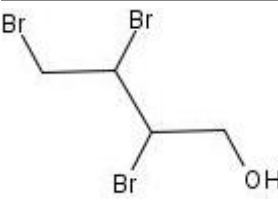
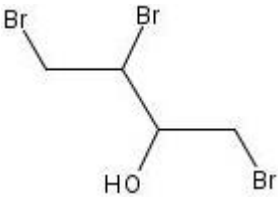
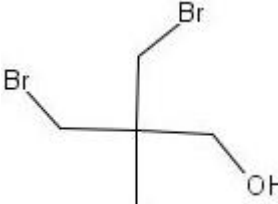
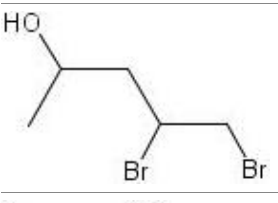
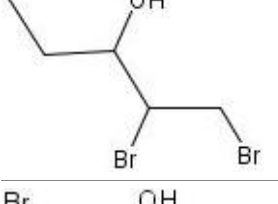
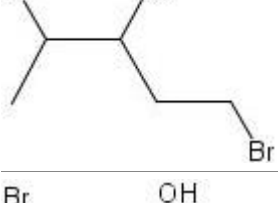
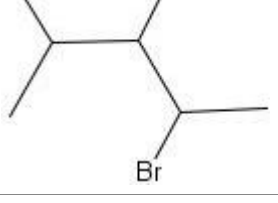
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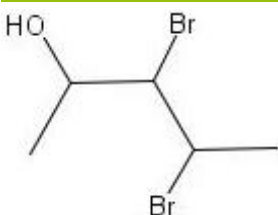
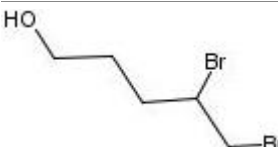
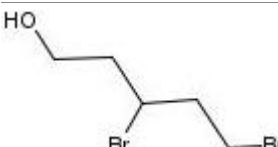
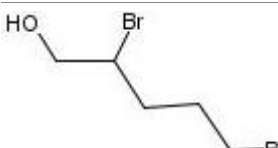
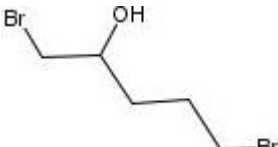
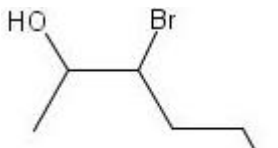

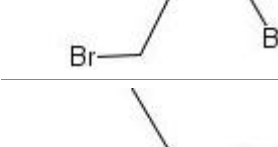
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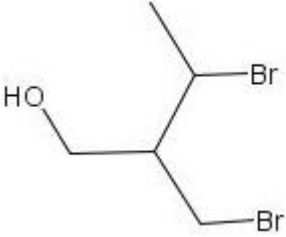
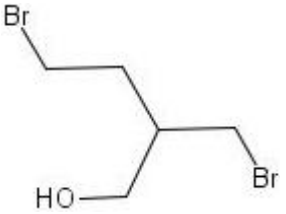
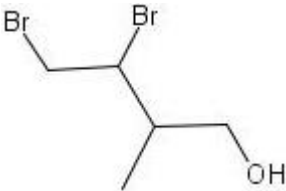
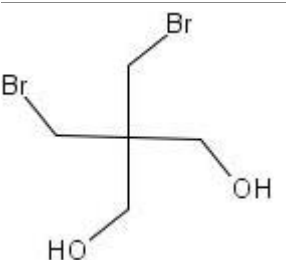
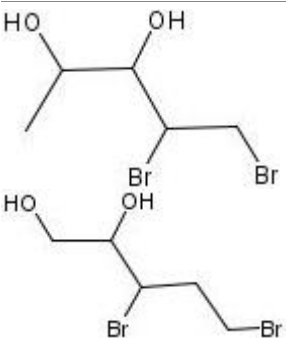
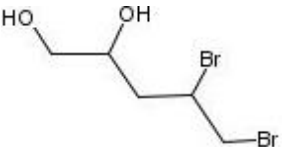
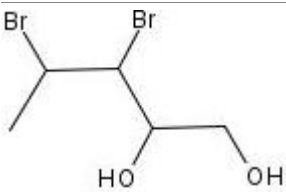
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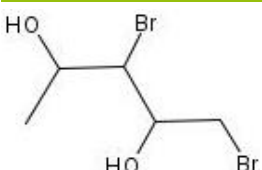
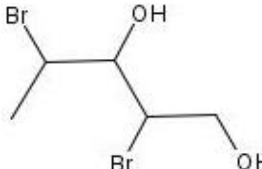
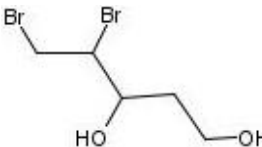
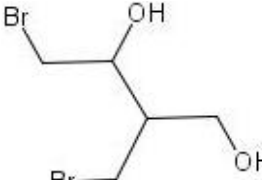
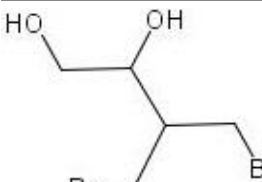
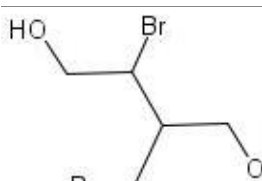
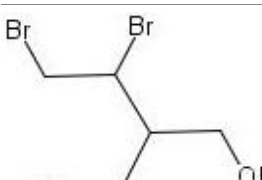
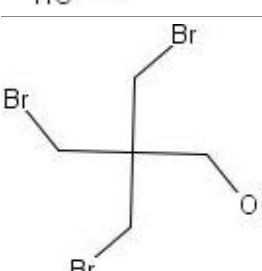
6. Appendix I: List of substances identified in the scope of the „small brominated alkyl alcohols“ group

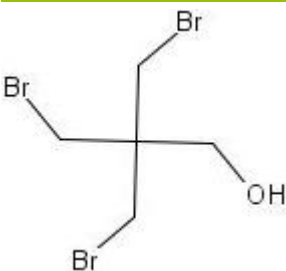
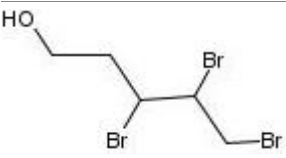
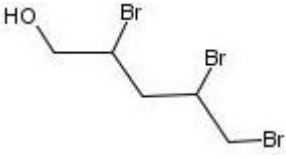
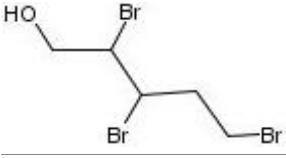
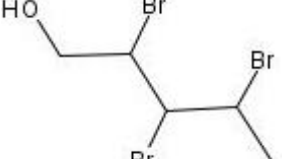
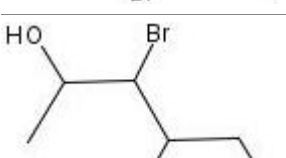
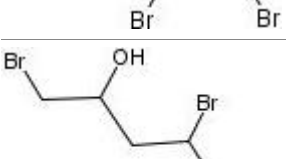
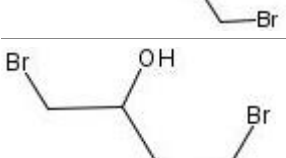
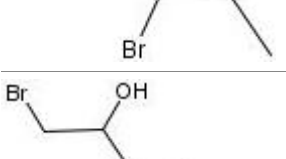
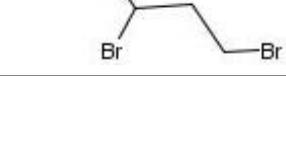
| Structure | CAS number | EC number | Name |
|---|-------------|-----------|---|
|  | 96-13-9 | 202-480-9 | 2,3-dibromopropan-1-ol, 2,3-dibromo-1-propanol |
|  | 96-21-9 | 202-489-8 | 1,3-dibromopropan-2-ol |
|  | 106023-63-6 | | 3-Bromo-2-(bromomethyl)- 1-propanol |
|  | 19398-47-1 | 243-029-6 | 1,4-dibromobutan-2-ol |
|  | 79033-40-2 | | 3,4-Dibromo-2-butanol |
|  | 4021-75-4 | | 2,3-dibromobutan-1-ol |
|  | 87018-30-2 | | 3,4-Dibromo-1-butanol |
|  | 35330-59-7 | | 3,4-Dibromo-1,2-butanediol |

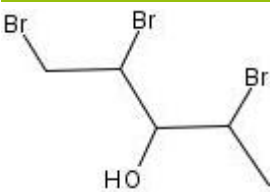
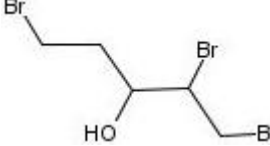
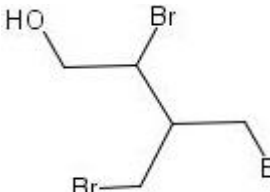
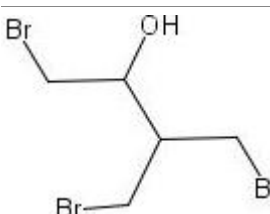
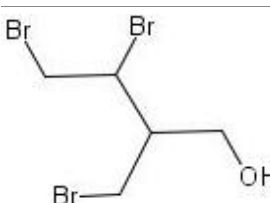
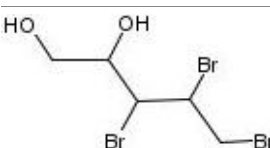
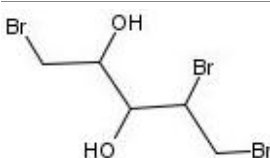
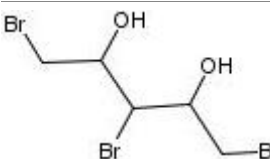
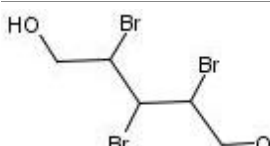
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|  | 14396-65-7 | 627-179-3 | 1,4-Dibromo-2,3-butanediol |
|  | 855236-37-2 | | 2,3,4-Tribromo-1-butanol |
|  | 87018-38-0 | | 1,2,4-Tribromo-3-butanol |
|  | 105100-80-9 | | 2,2-Bis(bromomethyl)-1-propanol |
|  | 213821-22-8 | | 4,5-Dibromo-2-pentanol |
|  | 408319-76-6 | | 1,2-Dibromo-3-pentanol |
|  | 159475-15-7 | | 1,4-dibromo-(R*,R*)-(9CI)-3-pentanol |
|  | 343268-04-2 | | 2,4-Dibromo-3-pentanol |

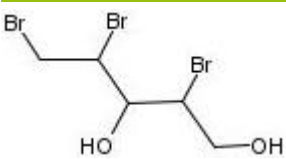
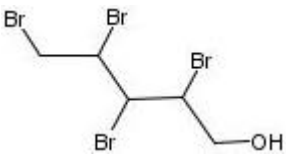
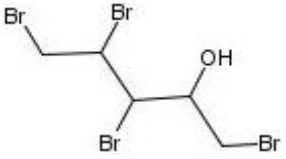
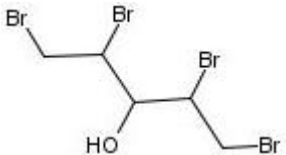
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|  | 76377-07-6 | | 3,4-Dibromo-(2R*,3S*,4S*)-(9CI)-2-pentanol |
|  | 59287-66-0 | | 4,5-Dibromo-1-pentanol |
|  | No CAS | | |
|  | 856991-78-1 | | 2,5-Dibromo-1-pentanol |
|  | 100606-66-4 | | 2-Pentanol, 1,5-dibromo- |
|  | 213821-20-6 | | 2,5-Dibromo-2-pentanol |
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|  | No CAS | | |

| Structure | CAS number | EC number | Name |
|---|------------|-----------|--|
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|  | 98069-26-2 | | 4-Bromo-2-(bromomethyl)-1-butanol |
|  | No CAS | | |
|  | 3296-90-0 | 221-967-7 | 2,2-bis(bromomethyl)propane-1,3-diol Synonyms: Dibromo-neopentyl-glycol |
|  | No CAS | | |
|  | No CAS | | |
|  | No CAS | | |

| Structure | CAS number | EC number | Name |
|---|------------|-----------|---|
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|  | No CAS | | |
|  | No CAS | | |
|  | 44804-46-8 | | 4-Bromo-2-(bromomethyl)-1,3-butanediol |
|  | No CAS | | |
|  | No CAS | | |
|  | No CAS | | |
|  | 1522-92-5 | 622-370-8 | 3-Bromo-2,2-bis(bromomethyl)-1-propanol |

| Structure | CAS number | EC number | Name |
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|  | 36483-57-5 | 253-057-0 | 2,2-dimethylpropan-1-ol, tribromo derivative Synonym: Tribromoneopentyl alcohol |
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