

Tetrabromobisphenol A bis(2,3-dibromopropyl ether)
[21850-44-2]

Review of Toxicological Literature

November 2002

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Prepared for

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Executive Summary

Nomination

Tetrabromobisphenol A bis(2,3-dibromopropyl ether) (TBBPA-DBPE) was nominated for toxicological characterization by the National Institute of Environmental Health Sciences (NIEHS) based on studies of 2,3-dibromo-1-propanol (DBP) and the DBP-based flame retardant tris(2,3-dibromopropyl)phosphate (TBP) that showed clear evidence of carcinogenicity in all sex-species combinations in two-year dermal and feed studies, respectively, conducted by the National Toxicology Program (NTP). Out of 32 compounds identified with the DBP substructure, only TBBPA-DBPE was found to be currently in production and use.

Nontoxicological Data

Production Information

TBBPA-DBPE is supplied by TCI America (Portland, OR) and Aldrich Chemical Company, Inc. (Milwaukee, WI). It is available from Ameribrom, Inc. as FR-720. Great Lakes Chemical Corporation sells TBBPA-DBPE as PE-68 in blends (e.g., with antimony oxide) for formulation with polypropylene (PP).

Tetrabromobisphenol A (TBBPA) is used to produce PE-68 by Great Lakes Chemical Corporation. No process information was provided. An aggregate production volume range of 1-10 million pounds was reported in non-confidential production volume information submitted by companies for chemicals under the 1998 TSCA Inventory Update Rule (<http://www.epa.gov/oppt/iur/iur98/index.htm>). Other production or import volumes were not available. It was, however, reported that the market for the compound as a V-2 flame retardant for high-impact polystyrene (HIPS) has been growing at a steady rate.

Uses

TBBPA-DBPE is an additive flame retardant for polyolefins and polymers, including PP, high-density polyethylene (HDPE), and low-density polyethylene (LDPE). The substance is also used in fabricated plastic sheet materials for application in the formation of a part of many electrical cabinets. As Saytex[®] HP-800A flame retardant, the product is used in textiles, paints, and hot melts. Additionally, it and its granular form HP-800AG are used in PP and HIPS applications such as pipes, water barriers, kitchen hoods, household, and in TV, hifi-audio, and electronics. Ameribrom's FR-720 is also used for PP.

Environmental Occurrence and Persistence

In biodegradation tests, TBBPA-DBPE was negative. Only small amounts of TBBPA-DBPE were found to bioaccumulate in carp.

Regulatory Status

TBBPA-DBPE is listed in the Toxic Substances Control Act (TSCA) Inventory. The compound was also indexed in TOXLINE records for "Polyhalogenated Dibenzo-*p*-dioxins-dibenzofurans Testing and Reporting Requirements Under TSCA."

Human Data

Human exposure to TBBPA-DBPE may result during manufacture, use as a flame retardant, and through contact with products containing the substance. Three cases of workers developing skin and/or eye irritation have been reported. The symptoms occurred while using thermoplastic resin formulations containing TBBPA-DBPE as an additive.

Toxicological Data

Great Lakes Chemical Corporation has submitted unpublished health and safety studies to the Environmental Protection Agency (EPA) [TSCATS Section 8(e) submissions] for four formulations containing TBBPA-DBPE, including Ames tests results.

Acute Exposure

The oral and dermal LD₅₀ (lethal dose for 50% of test animals) values for TBBPA-DBPE were reported to be >20 g/kg (21 mmol/kg) in mice.

Short-term and Subchronic Exposure

Mice administered TBBPA-DBPE (200 or 2000 mg/kg [0.212 or 2.119 mmol/kg]) daily in the diet for 90 days exhibited no abnormal gross pathological symptoms and had no deaths.

Genotoxicity

In *Salmonella typhimurium* strains TA100 and TA1535, TBBPA-DBPE (dose[s] not provided) was mutagenic in the absence and presence of metabolic activation. Additionally, it was positive for mutagenic activity in strain TA98 in the absence of metabolic activation.

In a rat unscheduled DNA synthesis assay, TBBPA-DBPE (10, 50, 100, 500, and 1000 µg/mL [11, 53, 106, 530, and 1059 µM]) was negative. Furthermore, the compound (5, 17, 50, 170, and 500 µg/mL [5, 18, 53, 180, and 530 µM]) failed to induce sister chromatid exchanges (SCEs) in Chinese hamster ovary (CHO) cells in the presence and absence of metabolic activation.

Other Data

No data were available regarding chemical disposition, metabolism, or toxicokinetics; chronic toxicity; synergistic/antagonistic effects; cytotoxicity; reproductive or teratological effects; carcinogenicity; or immunotoxicity.

Structure-Activity Relationships

A literature search was also conducted to identify other flame retardants with the 2,3-dibromo-1-propanol substructure. Data on the following compounds are presented due to the availability of toxicity information: acute toxicity, subchronic or short-term toxicity, carcinogenicity, and genotoxicity.

2,3-Dibromo-1-propanol (DBP) [96-13-9]

DBP, a flame retardant, is also an intermediate in the preparation of tris(2,3-dibromopropyl)phosphate (TBP) (toxicity information provided below). In children wearing pajamas treated with TBP, DBP was detected in the urine.

Acute Toxicity: DBP is irritating to the skin, eyes, mucous membranes, and the upper respiratory tract. An intraperitoneal (i.p.) LD₅₀ value of 125 mg/kg was reported for mice. In rats, an oral toxicity value of 681 mg/kg was calculated; via inhalation, the LC₅₀ value was 9920 mg/m³ in the animals. During the four-hour inhalation study, the rats exhibited damage to sensory organs, somnolence, and dyspnea. In rabbits, the dermal LD₅₀ value was 316 mg/kg. In the eyes of rabbits, application of DBP (100 µL) for 24 hours produced severe irritation.

Subchronic or Short-term Toxicity: In rats, inhalation of DBP (500 mg/m³) for four hours per day for three weeks intermittently produced somnolence, liver weight changes, and death. When applied to the skin (11505 mg/kg), changes in tubules (e.g., acute tubular necrosis) were observed.

Carcinogenicity: Dermal studies have been conducted in which B6C3F₁ mice and F344/N rats were treated with DBP (44, 88, 177, 375, or 750 mg/kg) five days per week for 16 days, 13 weeks, or from 36

to 55 weeks. In the chronic studies, there was clear evidence of carcinogenic activity in both sexes of both species.

The International Agency for Research on Cancer (IARC) concluded that "there is sufficient evidence in experimental animals for the carcinogenicity of 2,3-dibromopropan-1-ol." Its overall evaluation was the following: "2,3-Dibromopropan-1-ol is possibly carcinogenic to humans (Group 2B)."

Genotoxicity: DBP is a mutagenic metabolite of TBP. In the absence of exogenous metabolic activation, DBP was mutagenic in *S. typhimurium* strains TA98, TA100, and TA1535. It was also mutagenic in the mouse lymphoma assay. In CHO cells, it induced SCEs and chromosomal aberrations (CAs), while in *Drosophila melanogaster*, it induced sex-linked recessive lethal mutations and reciprocal translocations. DBP was negative for mutagenic activity in an *in vivo* bone marrow micronucleus assay using male mice.

Tris(2,3-dibromopropyl)phosphate (TBP) [126-72-7]

TBP was the most widely used bromine- and phosphorus-containing flame retardant until its carcinogenic properties in animals led to its withdrawal from use in many countries. TBP was banned in 1977 by the U.S. Consumer Product Safety Commission and in several countries for use in children's clothing because of its potential carcinogenic activity and potential significant exposure through contact with such fabrics.

Chemical Disposition, Metabolism, and Toxicokinetics: In the rat, 86% of ¹⁴C-TBP was excreted in the form of metabolites in urine (58%), expired air (19% as ¹⁴CO₂), and feces (9%) five days after administration. Bis(2,3-dibromopropyl)phosphate (BBP) was detected in urine, feces, bile, and tissues, and DBP was identified in the urine and tissues. In addition, all tissues contained TBP-derived radioactivity; the kidney and colon, the tissues in which TBP was selectively toxic, had the highest concentrations. TBP was also found to be metabolized by rat liver microsomes; metabolites included BBP, bromide ion, and 2-bromoacrolein.

Carcinogenicity: When orally administered to B6C3F₁ mice, TBP (500 and 1000 ppm) produced renal tubular cell carcinoma and adenoma, squamous cell papilloma and carcinoma of the forestomach, hepatocellular carcinoma and adenoma, and bronchiolar/alveolar adenoma and carcinoma. The incidences of kidney and lung tumors were significantly increased in males, whereas the incidences of liver and lung tumors were significantly increased only in females. The incidences of squamous cell papillomas of the forestomach were significantly increased in both sexes. In a dermal study, TBP produced tumors of the skin, lung, forestomach, and oral cavity.

In Fischer 344 rats, TBP (50 and 100 ppm) in the feed caused kidney tubular cell adenomas; the incidences were significantly increased for both sexes and at both doses. Additionally, for males, the incidence of kidney tubular cell adenocarcinomas was significantly correlated with the dietary concentration of TBP. In another study of limited duration, benign colon tumors were found.

IARC's overall evaluation was the following: "Tris(2,3-dibromopropyl)phosphate is probably carcinogenic to humans (Group 2A)."

Genotoxicity: In *in vivo* assays, TBP induced micronuclei in bone marrow cells and sperm abnormalities in mice. In human cells *in vitro*, it induced SCEs and DNA damage. TBP transformed Syrian hamster embryo cells, as well as mouse C3H 10T1/2 cells. In cultured rodent cells, it induced CAs, SCEs, and mutations. In *Drosophila*, heritable translocations occurred, while in bacteria, DNA damage and mutation were observed.

Bis(2,3-dibromopropyl)phosphate (BBP) [5412-25-9]

BBP is a metabolite of TBP. Like TBP, it was banned in 1977 by the U.S. Consumer Product Safety Commission and in several countries for use in children's clothing. In rats, oral administration of the compound produced tumors. In *S. typhimurium* strain TA100, it was mutagenic in the presence of metabolic activation.

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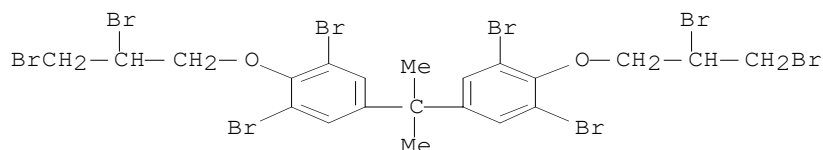
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1.0 Basis for Nomination

Tetrabromobisphenol A bis(2,3-dibromopropyl ether) (TBBPA-DBPE) was nominated by the National Institute of Environmental Health Sciences (NIEHS) for toxicological characterization based on studies of 2,3-dibromo-1-propanol (DBP) and the DBP-based flame retardant tris(2,3-dibromopropyl)phosphate (TBP) that showed clear evidence of carcinogenicity in all sex-species combinations in two-year dermal and feed studies, respectively, conducted by the National Toxicology Program (NTP). Out of 32 compounds identified with the DBP substructure, only TBBPA-DBPE was found to have substantial evidence of U.S. production and use.

2.0 Introduction

Tetrabromobisphenol A bis(2,3-dibromopropyl ether) (TBBPA-DBPE)
[21850-44-2]



2.1 Chemical Identification and Analysis

TBBPA-DBPE [C₂₁H₂₀Br₈O₂; mol. wt. = 943.9] is also called the following:

Propane, 2,2-bis[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]- (8CI)
 Benzene, 1,1'-(1-methylethylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)- (9CI)
 1,1'-Isopropylidenebis[3,5-dibromo-4-(2,3-dibromopropoxy)benzene]
 2,2-Bis[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]propane
 2,2-Bis[4-(2,3-dibromopropoxy)-3,5-dibromophenyl]propane
 2,2-Bis[4-(2,3-dibromopropoxy)-3,5-dibromophenyl]propane
 2,2-Bis[[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]]propane
 3,3',5,5'-Tetrabromobisphenol A bis(2,3-dibromopropyl) ether
 4,4'-Isopropylidenebis[2,6-dibromo-1-(2,3-dibromopropoxy)benzene]
 Bis(2,3-dibromopropoxy)tetrabromobisphenol A
 Bromkal 66-8
 D 5532
 Dibromopropydian
 FG 3100
 Fire Guard 3100
 Flame Cut 121K
 Flame Cut 121R
 GX 5532
 PE 68
 Pyroguard SR 720
 SR 720
 Tetrabromobisphenol A 2,3-dibromopropyl ether
 Tetrabromobisphenol A dibromopropyl ether

Sources: IPCS (1995); Registry (2002)

No analytical techniques were available.

2.2 Physical-Chemical Properties

Property	Information	Reference
TBBPA-DBPE		
Physical State	crystalline or powdered white/off-white solid	IPCS (1995)
% Bromine	68	
Odor	slight odor	
Melting Point (°C)	90-100; decomposition at >270	
Specific Gravity (g/cm ³)	0.7-0.9	
Water Solubility (g/L)	1 @ 25 °C*	
Saytex[®] HP-800A		
Physical State	white powder; dust-free granules	Albemarle (2002a)
% Bromine, theoretical	67.8	
Melting Point (°C)	108-120	
Specific Gravity (kg/L)	2.13	
Bulk Density		
packed (g/100 mL)	84.3	
aerated (g/100 mL)	79.8	
Soluble in:	acetone, methanol, and toluene	
Saytex[®] HP-800AG		
Physical State	dust-free white granules	Albemarle (2002b)
% Bromine, theoretical	64.4	
Melting Point (°C)	95-120	
Specific Gravity (kg/L)	1.127	

* noted by IPCS (1995) to be too high a value

Saytex[®] HP-800A is an additive flame retardant combining aromatic bromine with aliphatic bromine. Saytex[®] HP-800AG is its dust-free granular form. Both products are usually used with antimony trioxide for maximum retardant performance (Albemarle, 2002a,b). Used as a lubricant or demolding compound in high-impact polystyrene (HIPS), zinc stearates produce premature decomposition and discoloration in TBBPA-DBPE products (Great Lakes Chem. Corp., 2001b).

2.3 Commercial Availability

TBBPA-DBPE is supplied by TCI America (Portland, OR) and Aldrich Chemical Company, Inc. (Milwaukee, WI) (Salor, 2001; TCI American, 2000 [both in the CHEMCATS database]). It is available from Ameribrom, Inc. as FR-720 (DSBG, undated; Wigotsky, 2001). Great Lakes Chemical Corporation, the leading producer of certain specialty chemicals for applications including flame retardants, sells PE-68 in blends (e.g., with antimony oxide) for formulation with polypropylene (PP) (Great Lakes Chem. Corp., 2001a,b). To overcome the problem of plastics degradation due to remaining reactive groups in plastics compounded with TBBPA-DBPE, the formulations contain alkyl end groups to reduce reactivity (Flame Retard. News, 1996a).

TBBPA-DBPE is available only in Europe from Albemarle Corporation as Saytex[®] HP-800A (Albemarle, undated). The company sells it in 25-kg paper bags and in 500-kg bags (Albemarle, 2002a). Saytex[®] HP-800AG is available in 25-kg polyethylene bags (Albemarle, 2002b).

3.0 Production Processes

TBBPA is used to produce PE-68 by Great Lakes Chemical Corporation (Flame Retard. News, 1992). No process information was provided.

4.0 Production and Import Volumes

An aggregate production volume range of 1-10 million pounds was reported in non-confidential production volume information submitted by companies for chemicals under the 1998 TSCA Inventory Update Rule (<http://www.epa.gov/oppt/iur/iur98/index.htm>). Other production or import volumes were not available. The market for the compound as a V-2 flame retardant for HIPS has been growing at a steady rate (Jpn. Chem. Week, 1998).

5.0 Uses

TBBPA-DBPE is a substitute for the flame retardant decabromodiphenyl oxide (DBDPO), the use of which was initially suspended due to environmental problems (Jpn. Chem. Week, 1998). It is an additive flame retardant for polyolefins and polymers, including PP, high-density polyethylene (HDPE), and low-density polyethylene (LDPE) (OECD, 1994). The substance is also used in fabricated plastic sheet materials for application in the formation of a part of many electrical cabinets (Flame Retard. News, 1996b).

As Saytex[®] HP-800A flame retardant, the product is used in textiles, paints, and hot melts (Albemarle, undated). Additionally, it and its granular form HP-800AG are used in PP and HIPS applications such as pipes, water barriers, kitchen hoods, household, and in TV, hifi-audio, and electronics (Albemarle, 2002a,b). Ameribrom's FR-720 is also used for PP (DSBG, undated; Wigotsky, 2001).

6.0 Environmental Occurrence and Persistence

In biodegradation tests, TBBPA-DBPE was negative. Only small amounts of TBBPA-DBPE were found to bioaccumulate in carp (Great Lakes Chem. Corp., 1987; cited by IPCS, 1995).

7.0 Human Exposure

Human exposure to TBBPA-DBPE may result during its manufacture, use as a flame retardant, and through contact with products (e.g., thermoplastic resin formulations) containing the substance as an additive.

8.0 Regulatory Status

TBBPA-DBPE is listed in the Toxic Substances Control Act (TSCA) Inventory; Section 4 of the Act applies to the chemical (TSCA INV, 2002). The compound was also indexed in TOXLINE records for "Polyhalogenated Dibenzo-*p*-dioxins-dibenzofurans Testing and Reporting Requirements Under TSCA" (Johnson et al., 1989, 1990; Remmers et al., 1991).

9.0 Toxicological Data

9.1 General Toxicology

Great Lakes Chemical Corporation has submitted unpublished health and safety studies to the Environmental Protection Agency (EPA) [TSCATS Section 8(e) submissions] for four formulations containing TBBPA-DBPE, including Ames tests results.

9.1.1 Human Data

Three cases of workers developing skin and/or eye irritation have been reported (Great Lakes Chemical Corporation TSCA 8(e) report [8EHQ-0699-14475]). The symptoms occurred while

using thermoplastic resin formulations containing TBBPA-DBPE as an additive (Pestic. Toxic Chem. News, 1999).

9.1.2 Chemical Disposition, Metabolism, and Toxicokinetics

No data were available.

9.1.3 Acute Exposure

The oral and dermal LD₅₀ values for TBBPA-DBPE were reported to be >20 g/kg (21 mmol/kg) in mice (Great Lakes Chem. Corp., 1987; cited by IPCS, 1995).

9.1.4 Short-term and Subchronic Exposure

Mice administered TBBPA-DBPE (200 or 2000 mg/kg [0.212 or 2.119 mmol/kg]) daily in the diet for 90 days exhibited no abnormal gross pathological symptoms and had no deaths (Great Lakes Chem. Corp., 1987; cited by IPCS, 1995).

9.1.5 Chronic Exposure

No data were available.

9.1.6 Synergistic/Antagonistic Effects

No data were available.

9.1.7 Cytotoxicity

No data were available.

9.2 Reproductive and Teratological Effects

No data were available.

9.3 Carcinogenicity

No data were available.

9.4 Initiation/Promotion Studies

No data were available.

9.5 Anticarcinogenicity

No data were available.

9.6 Genotoxicity

In *Salmonella typhimurium* strains TA100 and TA1535, TBBPA-DBPE (dose[s] not provided) was mutagenic in the absence and presence of metabolic activation. Additionally, it was positive for mutagenic activity in strain TA98 in the absence of metabolic activation. The results indicated that rat liver S9 mix converted the substance to a less mutagenic form (Brusick, 1982; cited by IPCS, 1995).

In a rat unscheduled DNA synthesis assay, TBBPA-DBPE (10, 50, 100, 500, and 1000 µg/mL [11, 53, 106, 530, and 1059 µM]) was negative (Cavagnaro and Sernau, 1984; cited by IPCS, 1995). Furthermore, the compound (5, 17, 50, 170, and 500 µg/mL [5, 18, 53, 180, and 530

μM]) failed to induce sister chromatid exchanges (SCEs) in Chinese hamster ovary (CHO) cells in the presence and absence of metabolic activation (Cavagnaro and Cortina, 1984; cited by IPCS, 1995).

9.7 Cogenotoxicity

No data were available.

9.8 Antigenotoxicity

No data were available.

9.9 Immunotoxicity

No data were available.

9.10 Other Data

No other data were available.

10.0 Structure-Activity Relationships

A search was conducted on flame retardants with the 2,3-dibromo-1-propanol substructure. The search description and summary are provided in Appendix B. In this section, brief toxicity data, especially carcinogenicity and genotoxicity, are presented for the following compounds: 2,3-dibromo-1-propanol, tris(2,3-dibromopropyl)phosphate, and bis(2,3-dibromopropyl)phosphate. [Note: Dose(s) and/or exposure period are given when provided in the sources.]

2,3-Dibromo-1-propanol (DBP) [96-13-9]

DBP, a flame retardant, is also an intermediate in the preparation of tris(2,3-dibromopropyl)phosphate (TBP) (toxicity information provided below). In children wearing pajamas treated with TBP, DBP was detected in the urine (IARC, 2000).

Acute Toxicity: DBP is irritating to the skin, eyes, mucous membranes, and the upper respiratory tract. An intraperitoneal (i.p.) LD₅₀ value of 125 mg/kg was reported for mice (Radian, 2001). In rats, an oral toxicity value of 681 mg/kg was calculated; via inhalation, the LC₅₀ value was 9920 mg/m³ in the animals. During the four-hour inhalation study, the rats exhibited damage to sensory organs (not otherwise specified), somnolence, and dyspnea. In rabbits, the dermal LD₅₀ value was 316 mg/kg. In the eyes of rabbits, application of DBP (100 μL) for 24 hours produced severe irritation (RTECS, 1999).

Subchronic or Short-term Toxicity: In rats, inhalation of DBP (500 mg/m³) for four hours per day for three weeks intermittently produced somnolence, liver weight changes, and death. When applied to the skin (11505 mg/kg), changes in tubules, including acute renal failure and acute tubular necrosis, were observed (RTECS, 1999).

Carcinogenicity: Dermal studies have been conducted in which B6C3F₁ mice and F344/N rats were treated with DBP (44, 88, 177, 375, or 750 mg/kg) five days per week for 16 days, 13 weeks, or from 36 to 55 weeks. In the chronic studies, there was clear evidence of carcinogenic activity in both sexes of both species (NTP, 1993). (Full details of *all* studies are available at <http://ntp-server.niehs.nih.gov/htdocs/LT-studies/tr400.html>.) The International Agency for

Research on Cancer (IARC) concluded that "there is sufficient evidence in experimental animals for the carcinogenicity of 2,3-dibromopropan-1-ol." Its overall evaluation was the following: "2,3-Dibromopropan-1-ol is possibly carcinogenic to humans (Group 2B)" (IARC, 2000).

Genotoxicity: DBP is a mutagenic metabolite of TBP (Radian, 2001). In the absence of exogenous metabolic activation, DBP was mutagenic in *S. typhimurium* strains TA98, TA100, and TA1535. It was also mutagenic in the mouse lymphoma assay, inducing trifluorothymidine resistance in L5178Y cells. In CHO cells, it induced SCEs and chromosomal aberrations (CAs), while in *Drosophila melanogaster*, it induced sex-linked recessive lethal mutations and reciprocal translocations. DBP was negative for mutagenic activity in an *in vivo* bone marrow micronucleus assay using male mice (NTP, 1993). Studies in hamster lung and rat liver and other rat cell types have also been performed (RTECS, 1999).

Tris(2,3-dibromopropyl)phosphate (TBP) [126-72-7]

TBP was the most widely used bromine- and phosphorus-containing flame retardant until its carcinogenic properties in animals led to its withdrawal from use in many countries. TBP was banned in 1977 by the U.S. Consumer Product Safety Commission and in several countries for use in children's clothing because of its potential carcinogenic activity and potential significant exposure through contact with such fabrics (IPCS, 1997).

Chemical Disposition, Metabolism, and Toxicokinetics: In the rat, 86% of ¹⁴C-TBP was excreted in the form of metabolites in urine (58%), expired air (19% as ¹⁴CO₂), and feces (9%) five days after administration. Bis(2,3-dibromopropyl)phosphate (BBP) was detected in urine, feces, bile, and tissues, and DBP was identified in the urine and tissues. In addition, all tissues contained TBP-derived radioactivity; the kidney and colon, the tissues in which TBP was selectively toxic, had the highest concentrations (Lynn et al., 1982).

TBP was also found to be metabolized by rat liver microsomes. Metabolites included BBP, bromide ion, and 2-bromoacrolein; the rates of formation for the first two compounds were increased in microsomes from phenobarbital-pretreated rats versus those from untreated rats (Söderlund et al., 1984).

Carcinogenicity: When orally administered to B6C3F₁ mice, TBP (500 and 1000 ppm) produced renal tubular cell carcinoma and adenoma, squamous cell papilloma and carcinoma of the forestomach, hepatocellular carcinoma and adenoma, and bronchiolar/alveolar adenoma and carcinoma. The incidences of kidney and lung tumors were significantly increased in males, whereas the incidences of liver and lung tumors were significantly increased only in females. The incidences of squamous cell papillomas of the forestomach were significantly increased in both sexes (NCI, 1978). In a dermal study, TBP produced tumors of the skin, lung, forestomach, and oral cavity (IARC, 1999).

In Fischer 344 rats, TBP (50 and 100 ppm) in the feed caused kidney tubular cell adenomas; the incidences were significantly increased for both sexes and at both doses. Additionally, for males, the incidence of kidney tubular cell adenocarcinomas was significantly correlated with the dietary concentration of TBP (NCI, 1978). In another study of limited duration, benign colon tumors were found (IARC, 1999).

IARC concluded that "there is inadequate evidence in humans for the carcinogenicity of tris(2,3-dibromopropyl) phosphate" but that "there is sufficient evidence in experimental animals for the carcinogenicity of tris(2,3-dibromopropyl)phosphate." The agency's overall evaluation was the following: "Tris(2,3-dibromopropyl)phosphate is probably carcinogenic to humans (Group 2A)" (IARC, 1999).

Genotoxicity: In *in vivo* assays, TBP induced micronuclei in bone marrow cells and sperm abnormalities in mice. In human cells *in vitro*, it induced SCEs and DNA damage. TBP transformed Syrian hamster embryo cells, as well as mouse C3H 10T1/2 cells. In cultured rodent cells, it induced CAs, SCEs, and mutations. In *Drosophila*, heritable translocations occurred, while in bacteria, DNA damage and mutation were observed (IARC, 1987).

Bis(2,3-dibromopropyl)phosphate (BBP) [5412-25-9]

BBP is a metabolite of TBP. Like TBP, it was banned in 1977 by the U.S. Consumer Product Safety Commission and in several countries for use in children's clothing (IPCS, 1997). In rats, oral administration of the compound produced tumors [not specified in summary] (IARC, 1999). In *S. typhimurium* strain TA100, it was mutagenic in the presence of metabolic activation (Lynn et al., 1982).

11.0 Online Databases and Secondary References

11.1 Online Databases

National Library of Medicine Databases

EMIC and EMICBACK (Environmental Mutagen Information Center)

STN International Files

AGRICOLA	CHEMCATS	NIOSHTIC
BIOSIS	EMBASE	PROMT
BIOTECHNO	ESBIOBASE	Registry
CA	LIFESCI	RTECS
CANCERLIT	MEDLINE	TOXCENTER

TOXLINE includes the following subfiles:

Toxicity Bibliography	TOXBIB
International Labor Office	CIS
Hazardous Materials Technical Center	HMTC
Environmental Mutagen Information Center File	EMIC
Environmental Teratology Information Center File (continued after 1989 by DART)	ETIC
Toxicology Document and Data Depository	NTIS
Toxicological Research Projects	CRISP
NIOSHTIC [®]	NIOSH
Pesticides Abstracts	PESTAB
Poisonous Plants Bibliography	PPBIB
Aneuploidy	ANEUPL
Epidemiology Information System	EPIDEM

Toxic Substances Control Act Test Submissions	TSCATS
Toxicological Aspects of Environmental Health	BIOSIS
International Pharmaceutical Abstracts	IPA
Federal Research in Progress	FEDRIP
Developmental and Reproductive Toxicology	DART

Databases Available on the Internet

Code of Federal Regulations (CFR), National Archives and Records Administration

In-House Databases

Current Contents on Diskette[®]

The Merck Index, 1996, on CD-ROM

11.2 Secondary References

No secondary sources were used.

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720.pdf++%22+3+dibromopropyl%22+-phosphate+-phosphat&hl=e (html version of [http://www.deadseabromine.com/Brome/Brome.nsf/viewGetMain/Product263~40/\\$file/FR-720.pdf](http://www.deadseabromine.com/Brome/Brome.nsf/viewGetMain/Product263~40/$file/FR-720.pdf). Last accessed on December 21, 2001.

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Acknowledgements

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Appendix A: Units and Abbreviations

°C = degrees Celsius

µg/mL = microgram(s) per milliliter

µM = micromolar

BBP = bis(2,3-dibromopropyl)phosphate

CA = chromosomal aberration

CHO = Chinese hamster ovary

DBP = 2,3-dibromo-1-propanol

g = gram(s)

g/L = gram(s) per liter

HIPS = high-impact polystyrene

IARC = International Agency for Research on Cancer

IPCS = International Programme on Chemical Safety

kg = kilogram(s)

kg/L = kilogram(s) per liter

L = liter(s)

LD₅₀ = lethal dose for 50% of test animals

mg/kg = milligram(s) per kilogram

mg/m³ = milligram(s) per cubic meter

mmol = millimole(s)

mmol/kg = millimole(s) per kilogram

mol. wt. = molecular weight

NCI = National Cancer Institute

NTP = National Toxicology Program

OECD = Organisation for Economic Co-operation and Development

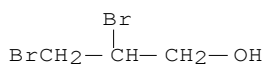
PP = polypropylene

SCE = sister chromatid exchange

TBBPA-DBPE = tetrabromobisphenol A bis(2,3-dibromopropyl ether)

TBP = tris(2,3-dibromopropyl)phosphate

Appendix B: Search Description and Summary of Results for Selected Flame Retardants with the 2,3-Dibromo-1-propanol substructure



2,3-Dibromo-1-propanol

Search Description

Rationale for inclusion in the searches:

- CAS Registry Number (CAS RN) identified plus one or more of the following:
- Listed in IPCS Environmental Health Criteria (EHC) Nos. 172, 173, or 192 (or a similar compound is listed).
- Listed in the TSCA Inventory.
- Records in RTECS and/or other biomedical databases.
- Numerous CA records. (Most compounds with fewer than about 10 CA records were excluded.)

In all selected compounds, the substructure was linked by an oxygen atom (ether or ester linkages) to the rest of the molecule. Tris(2,3-dibromopropyl) phosphate (L736) was not included in the searches.

The major search was conducted simultaneously in STN International databases MEDLINE, CANCERLIT, AGRICOLA, NIOSHTIC, BIOTECHNO, EMBASE, ESBIOBASE, IPA, BIOSIS, TOXCENTER, and PASCAL on June 5, 2002, using CAS RNs and name fragments. (See search statements below for several of the compounds.) When individual results were combined and duplicates removed, the numbers of records per database were the following:

ANSWERS '1-22' FROM FILE MEDLINE	Total 22/13/4/1
ANSWERS '23-24' FROM FILE CANCERLIT	2/2/-/-
ANSWERS '25-26' FROM FILE AGRICOLA	2/1/-/-
ANSWERS '27-30' FROM FILE NIOSHTIC	4/2/-/-
ANSWERS '31-33' FROM FILE EMBASE	3/-/2/1
ANSWERS '34-35' FROM FILE IPA	2/-/-/-
ANSWERS '36-42' FROM FILE BIOSIS	7/1/1/-
ANSWERS '43-67' FROM FILE TOXCENTER	25/1/3/2
ANSWER '68' FROM FILE LIFESCI	1/-/-/-
	<hr/>
	68/20/10/4
Separate TOXLINE search 6/6/02	/5/3/5

In the array of database totals above, the first number is the total from the simultaneous search; the second number is for records that matched citations on bis(2,3-dibromopropyl) phosphate(L737) or its salts in EHC No. 173 (IPCS, 1995b); the third number is for records on L737 or its salts not cited in IPCS (1995b); and the fourth number is for records on other derivatives. Publications on L737 cited in IPCS (1995b) will be summarized in this search package only if other selected compounds were tested.

A TOXLINE search using "tetrabromobisphenol A" AND dibromopropyl found 15 results, which included 8 TSCA test submissions. Generally, only the CAS RN was used as the search term in the TOXLINE searches. The TSCATS database on the Chemical Information Systems found more complete records for the compounds indicated below than the corresponding records in TOXLINE. The TSCA test submissions are not included in the TOXLINE tallies above.

None of the TSCA-listed compounds were found in the EPA Inventory Update Rule database. Other databases searched include CCRIS, DIOGENES (no results), PROMT, REGISTRY, RTECS, SANSS, TSCAINV, and TSCAPP. Product information was found at Internet web sites.

Summary of Results and Search Statements for Individual Compounds

The compounds, including 2,3-dibromo-1-propanol itself, are listed in this summary in order by the arbitrarily assigned ILS code. The boldfaced header separates the following information by semicolons: ILS code, EHC No., numbers of records in CA/CAOLD, and whether listed in TSCA or not. EHC No. 172 corresponds to IPCS (1995a); EHC No. 173, IPCS (1995b); and EHC No. 192, IPCS (1997). The annotation CN means "complete name." Ten compounds are listed in the TSCA Inventory: L730-AC, L731, L732, L734, L737, and the five uncoded compounds on pages 19 and 20. The latter five have no entries in any database, including CA.

The references collected are organized into three groups of abstracts, the Registry records, the CHEMCATS records, the RTECS records, the TSCATS records for L730-AC and L731, the IPCS reviews, and miscellaneous individual references. The first group of abstracts are for those references cited in IPCS (1995b) on L737. The second group of abstracts are for references not cited in IPCS (1995b). The third group of abstracts are for compounds other than L737.

L730; -; 328/20; TSCA

RN 96-13-9 REGISTRY

CN 1-Propanol, 2,3-dibromo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1,2-Dibromopropan-3-ol

CN **2,3-Dibromo-1-propanol**

CN 2,3-Dibromopropyl alcohol

CN Brominex 257

CN DBP

CN DBP (flame retardant)

Carcinogenesis References:

NTP TR-400 (1993); Eustis et al. (1995); IARC (2000); *NTP Report on Carcinogens*, 10th ed. For a quick summary of other toxic effects for an SAR discussion, see the RTECS record, which summarizes multiple-dose studies, genotoxicity studies, and acute toxicity studies. [No other searches were done for L730.]

L730-AC; 192; 45/-; TSCA

RN 19660-16-3 REGISTRY

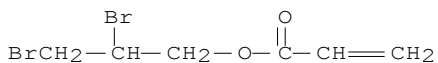
CN 2-Propenoic acid, 2,3-dibromopropyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1-Propanol, 2,3-dibromo-, acrylate (8CI)

CN Acrylic acid, 2,3-dibromopropyl ester (8CI)

OTHER NAMES:

CN **2,3-Dibromopropyl acrylate***Search Statements and Results for L730-AC:*

=> S 2(W)3(W)(DIBROMOPROPYL OR DIBROMOPROPOXY? OR DIBROMOPROPYLOXY?)

L1 884 2(W) 3(W)(DIBROMOPROPYL OR DIBROMOPROPOXY? OR DIBROMOPROPYLOXY?)

=> S L1(3A)(ACRYLIC OR ACRYLATE) OR 19660-16-3

L2 3 L1(3A)(ACRYLIC OR ACRYLATE) OR 19660-16-3

=> DUP REM L2 [Command = Remove duplicates]

L3 3 DUP REM L2 (0 DUPLICATES REMOVED)

ANSWERS '1-3' FROM FILE TOXCENTER

References:

TCI America, Ameribrom, Inc. (affiliated with Dead Sea Bromine Group, Israel), and Monomer-Polymer & Dajac Laboratories, Inc. were U.S. suppliers listed in the CHEMCATS database. Amounts sold were not given. Great Lakes Chemical Corporation submitted two 8(d) TSCA reports on 28-day toxicity studies in rats dosed orally with L730-AC. An initial submission by Great Lakes in 1984 covered acute oral and inhalation toxicity studies in rats; dermal toxicity and skin and eye irritation studies in rabbits; subchronic oral toxicity in rats (TD_{LO} given as 1680 mg/kg in RTECS), and genotoxicity in bacteria and yeast. IPCS (1997) (EHC No. 192) listed the acrylate as a flame retardant for acrylic resins. Lawson and Jurs (1990) clustered 143 acrylate esters, including L730-AC and L730 methacrylate (L730-MAC), in groups with similar chemical attributes "to simplify sampling for further toxicity screening." Zeiger et al. (1987) reported results from Salmonella tests with L730-AC (in RTECS record) and L730-MAC. CCRIS (1993) summarized the genotoxicity results: Positive in TA 100 and TA 1535 with metabolic activation by both rat liver and hamster liver S9. Also positive in TA 1535 without S9. Positive in TA 98 only with activation by hamster S9. Negative in TA 1537 with metabolic activation.

L730 ether; -; 8/2; Not TSCA

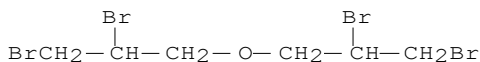
RN 59261-06-2 REGISTRY

CN Propane, 1,1'-oxybis[2,3-dibromo- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Ether, bis(2,3-dibromopropyl) (6CI)

OTHER NAMES:

CN **Bis(2,3-dibromopropyl) ether***References:*

Liepins and Pearce (1977) reviewed chemistry and toxicity of flame retardants, including L730 ether.

L730-FUM; -; 10/4; Not TSCA

L4 ANSWER 29 OF 29 REGISTRY COPYRIGHT 2002 ACS

RN 3925-73-3 REGISTRY

CN 2-Butenedioic acid (2E)-, bis(2,3-dibromopropyl) ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1-Propanol, 2,3-dibromo-, fumarate

CN 2-Butenedioic acid (E)-, bis(2,3-dibromopropyl) ester

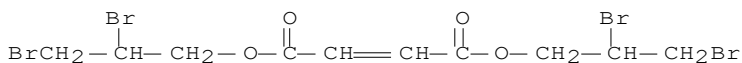
CN Fumaric acid, bis(2,3-dibromopropyl) ester (7CI, 8CI)

OTHER NAMES:

CN **Bis(2,3-dibromopropyl) fumarate**

CN FR 2

CN FR 2 (fire retardant)



L730-MAC; -; 20/5; Not TSCA.

RN 3066-70-4 REGISTRY

CN 2-Propenoic acid, 2-methyl-, 2,3-dibromopropyl ester (9CI) (CA INDEX NAME)

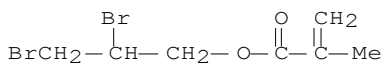
OTHER CA INDEX NAMES:

CN 1-Propanol, 2,3-dibromo-, methacrylate

CN Methacrylic acid, 2,3-dibromopropyl ester (6CI, 7CI, 8CI)

OTHER NAMES:

CN 2,3-Dibromopropyl methacrylate

*References:*

Salmonella tests by Zeiger et al. (1987) were the only data in RTECS. CCRIS (1993) summarized the Salmonella results. They were the same as described above for L730-AC except that L730-MAC was negative in TA 1535 without S9.

L730-TERE; (cf. L732); 8/1; Not TSCA

RN 7415-06-7 REGISTRY

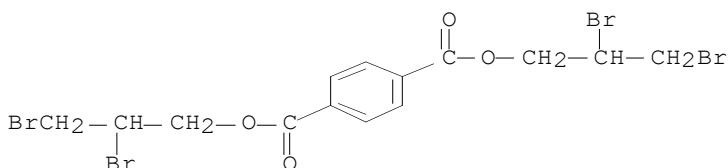
CN 1,4-Benzenedicarboxylic acid, bis(2,3-dibromopropyl) ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1-Propanol, 2,3-dibromo-, terephthalate (2:1)

CN Terephthalic acid, bis(2,3-dibromopropyl) ester (7CI, 8CI)

OTHER NAMES:

CN **Bis(2,3-dibromopropyl) terephthalate**

L731; 192; 260/-; TSCA

RN 21850-44-2 REGISTRY

CN Benzene, 1,1'-(1-methylethylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)-(9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Propane, 2,2-bis[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]- (8CI)

OTHER NAMES:

CN 1,1'-Isopropylidenebis[3,5-dibromo-4-(2,3-dibromopropoxy)benzene]

CN 2,2-Bis[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]propane

CN 2,2-Bis[4-(2,3-dibromopropoxy)-3,5-dibromophenyl]propane

CN 2,2-Bis[4-(2,3-dibromopropoxy)-3,5-dibromophenyl]propane

CN 2,2-Bis[[3,5-dibromo-4-(2,3-dibromopropoxy)]phenyl]propane

CN 3,3',5,5'-Tetrabromobisphenol A bis(2,3-dibromopropyl) ether

CN 4,4'-Isopropylidenebis[2,6-dibromo-1-(2,3-dibromopropoxy)benzene]

CN Bis(2,3-dibromopropoxy)tetrabromobisphenol A

CN Bromkal 66-8 CN D 5532

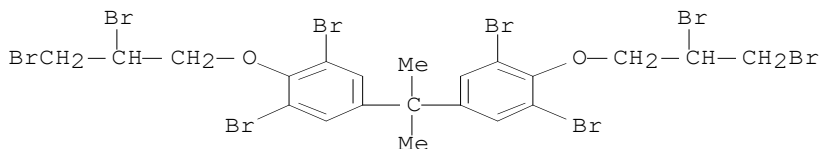
CN FG 3100 CN Fire Guard 3100

CN Flame Cut 121K CN Flame Cut 121R

CN GX 5532 CN PE 68

CN PE 68 (fireproofing agent) CN Pyroguard SR 720

CN SR 720 CN Tetrabromobisphenol A 2,3-dibromopropyl ether

CN **Tetrabromobisphenol A bis(2,3-dibromopropyl ether)***Search Statements and Results for L731:*

=> S TETRABROMOBISPHENOL(3A)L1

L4 6 TETRABROMOBISPHENOL(3A) L1

=> S BROMKAL(W)66(W)8

L5 0 BROMKAL(W) 66(W) 8

=> S 21850-44-2

L6 10 21850-44-2

=> S FIRE(W)GUARD(W)3100

L7 0 FIRE(W) GUARD(W) 3100

=> S FLAME(W)CUT(W)(121K OR 121R)

L8 0 FLAME(W) CUT(W)(121K OR 121R)

=> S PE(W)68

L9 10 PE(W) 68

=> S PYROGUARD(W)SR(W)720

L10 0 PYROGUARD(W) SR(W) 720

=> S SR(W)720

L11 6 SR(W) 720

=> S L4 OR L6 OR L9 OR L11

L12 31 L4 OR L6 OR L9 OR L11

=> DUP REM L12

PROCESSING COMPLETED FOR L12

L13 20 DUP REM L12 (11 DUPLICATES REMOVED)
ANSWERS '1-4' FROM FILE MEDLINE
ANSWER '5' FROM FILE NIOSHTIC
ANSWER '6' FROM FILE EMBASE
ANSWERS '7-8' FROM FILE IPA
ANSWER '9' FROM FILE BIOSIS
ANSWERS '10-20' FROM FILE TOXCENTER

The TOXLINE search used “tetrabromobisphenol A” AND dibromopropyl found 15 results, which included 8 TSCA test submissions. Twelve records were retrieved with the CAS RN alone.

References:

Albemarle (undated) listed L731 as a product available only in Europe. The database CHEMCATS lists TCI America and Aldrich Chemical Co. as U.S. suppliers; amounts are not indicated. Wigotsky (2001) reviewed the market for flame retardants in North America. Ameribrom's product line includes L731, trade name FR-720, for polypropylene.

Great Lakes Chemical Corporation expanded production of tetrabromobisphenol A at one of its two plants in El Dorado, Arkansas, in 1992. TBBPA is used to produce Great Lakes' L731 product, PE-68 (Flame Retardancy News, September 1992). Great Lakes Chemical Corporation (2001a,b) apparently makes its product PE-68 available in the United States, but it may be sold only in blends (e.g., with antimony oxide) for formulation with polypropylene. To overcome the problem of plastics degradation due to remaining reactive groups in plastics compounded with L731, Great Lakes provided formulations with alkyl end groups to reduce reactivity (Flame Retardancy News, 07-01-96). L731 is one of the flame retardants used in plastic sheets to fabricate “at least a part of many electric cabinets (Flame Retardancy News, 12-01-1996).

The Western European market for L731 in 1998 was 1,500 metric tons (Finnish Environ. Inst., undated). European and Israeli manufacturing plants have recently expanded production capacities for L731. One plant in The Netherlands was expected to have a capacity of 5,000 metric tons per year at start-up in 2000 (Comline Chem. Mater., 12 July 1999).

L731 is used as a flame retardant for polypropylene and styrenic-based products. Besides use in extrusion-grade polypropylene, L731 is used in high-density and low-density polyethylene (HDPE and LDPE) (OECD, 1994). Other sources just state it is used for polyolefins (IPCS, 1997).

Physical-chemical properties are given by Albemarle (2001), Danish EPA (1999), DSBG (undated), and OECD (1994). IPCS (1995a) (EHC No. 172 on Tetrabromobisphenol A and Its Derivatives) reviewed toxicity data for L731: positive in Salmonella tester strains TA 100 and TA 1535 without metabolic activation and negative in SCE and UDS assays. L731 was indexed in TOXLINE records for three related *Chemosphere* articles (Johnson et al., 1989, 1990; Remmers et al., 1991) on TSCA testing and reporting for PCDDs and PCDFs.

Worker reactions to L731 were described in a 1999 TSCA 8(e) report. Thermoplastic resin formulations containing L731 induced skin or eye irritation or both (Pesticide and Toxic Chemical News, 12 August 1999; Great Lakes Chemical Corp., 1999). In five other 8(e) submissions, Great Lakes provided process information and Ames test results for four formulations (TSCATS).

L732; 192; 7/1; TSCA

RN 7415-86-3 REGISTRY

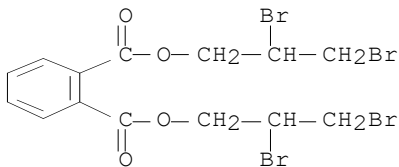
CN 1,2-Benzenedicarboxylic acid, bis(2,3-dibromopropyl) ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1-Propanol, 2,3-dibromo-, phthalate (2:1)

CN Phthalic acid, bis(2,3-dibromopropyl) ester (7CI, 8CI)

OTHER NAMES:

CN **Bis(2,3-dibromopropyl) phthalate***Search Statements and Results for L732:*

=> S L1(3A)(PHTHALIC OR PHTHALIC OR BENZENEDICARBOXYL?) OR 7415-86-3

L14 0 L1(3A)(PHTHALIC OR PHTHALIC OR BENZENEDICARBOXYL?) OR 7415-86-3

No TOXLINE records were retrieved using the CAS RN

References:

IPCS (1997) listed L732 as a flame retardant for which ITC had deferred testing.

L733; 192; 3/1; Not TSCA

RN 52434-59-0 REGISTRY

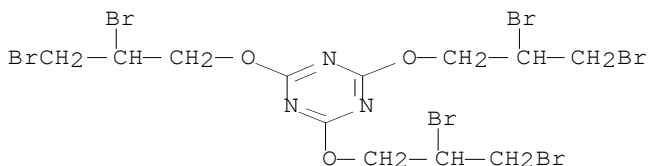
CN 1,3,5-Triazine, 2,4,6-tris(2,3-dibromopropoxy)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN *s*-Triazine, 2,4,6-tris(2,3-dibromopropoxy)- (6CI)

OTHER NAMES:

CN Tris(2,3-dibromopropyl) cyanurate

CN **2,4,6-Tris(2,3-dibromopropoxy)-1,3,5-triazine***Search Statements and Results for L733:*

=> S L1(6A)(TRIAZIN? OR CYANUR?) OR 52434-59-0

L15 0 L1(6A)(TRIAZIN? OR CYANUR?) OR 52434-59-0

=> S L1 AND (TRIAZIN? OR CYANUR?)

L16 5 L1 AND (TRIAZIN? OR CYANUR?)

=> DUP REM L16

L17 5 DUP REM L16 (0 DUPLICATES REMOVED)

ANSWER '1' FROM FILE CANCERLIT

ANSWERS '2-5' FROM FILE TOXCENTER

No TOXLINE records were retrieved using the CAS RN.

References:

IPCS (1997) and Danish EPA (1999) listed L733 as a brominated flame retardant for polypropylene.

L734; 192; 32/-; TSCA

RN 35109-60-5 REGISTRY

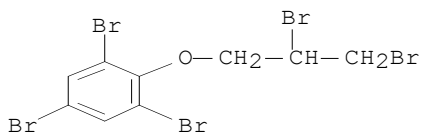
CN Benzene, 1,3,5-tribromo-2-(2,3-dibromopropoxy)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2,3-Dibromopropyl 2,4,6-tribromophenyl ether

CN **2,4,6-Tribromophenyl 2,3-dibromopropyl ether**

CN Bromkal 73-5PE

*Search Statements and Results for L734:*

=> S L1(6A)TRIBROMOPHENYL(6A)ETHER OR 35109-60-5 OR BROMKAL(W)73(W)5PE

L18 2 L1(6A) TRIBROMOPHENYL(6A) ETHER OR 35109-60-5 OR BROMKAL(W)
73(W) 5PE

=> DUP REM L18

L19 2 DUP REM L18 (0 DUPLICATES REMOVED)
ANSWERS '1-2' FROM FILE TOXCENTER

Use of the CAS RN on TOXLINE retrieved three records, presumably including the results reported by Zeiger et al. (1987) in the NTP Tech. Bull. in 1983.

References:

IPCS (1997) listed L734 as a commercial flame retardant. Huber and Ballschmiter (2001) identified L734 in a technical mixture using high-resolution gas chromatography/mass spectrometry. Sauer et al. (1997) identified L734 in sewer slimes in Germany.

L734b; -; 10/-; Not TSCA

RN 31394-74-8 REGISTRY

CN Benzene, tribromo(dibromopropoxy)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Ether, dibromopropyl tribromophenyl (8CI)

OTHER NAMES:

CN **Dibromopropyl tribromophenyl ether**

CN Tribromophenyl dibromopropyl ether



5 (D1—Br)

D1—O— Pr-n

References:

OECD (1994) listed “tribromophenoxy-dibromopropane” as a flame retardant for extrusion-grade polypropylene.

L735; -; 101/-; Not TSCA

RN 42757-55-1 REGISTRY

CN Benzene, 1,1'-sulfonylbis[3,5-dibromo-4-(2,3-dibromopropoxy)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4,4'-Bis(2,3-dibromopropoxy)-3,3',5,5'-tetrabromodiphenyl sulfone

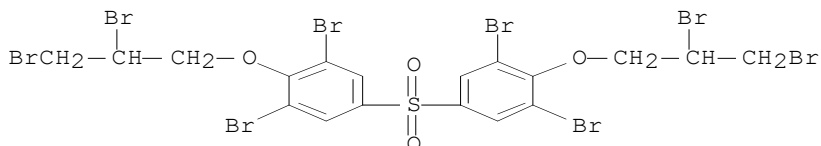
CN Bis[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl] sulfone

CN Flame Cut 161R

CN Nonnen 52

CN Nonnen PR 2

CN PR 2

CN **Tetrabromobisphenol S bis(2,3-dibromopropyl ether)***Search Statements and Results for L735:*

=> S TETRABROMOBISPHENOL(6A)L1(6A)ETHER OR 42757-55-1

L20 8 TETRABROMOBISPHENOL(6A) L1(6A) ETHER OR 42757-55-1

=> S L20 NOT L4

L21 3 L20 NOT L4

=> S L20 NOT L12

L22 0 L20 NOT L12

=> S 42757-55-1

L23 3 42757-55-1

No TOXLINE records (TOXLINE Special set) were retrieved using the CAS RN.

References:

Dettmer et al. (1999) in Germany found about 4% L735 in the backwall of a television cabinet made of polypropylene. L735 was stated to be commercially available in a *Flame Retardancy News* (April 2001) article describing "thin flame-resistant solid surface material" for wall cladding based on an acrylic polymer. Formulations were developed at DuPont in the United States. A Chinese supplier offered L735 in 25-kg bags; its web site gave product specifications and uses as pharmaceutical intermediate as well as flame retardant for "PV," polypropylene, and epoxy resins (jgbschem.com). Jiangsu Huading Refining Chemical Industry Co., Ltd. (undated) gave specifications for its L735 product.

L736 Tris(2,3-dibromopropyl) phosphate (CAS RN 126-72-7)

No search was done for L736; however, its carcinogenicity would need to be mentioned in the SAR section of a report.

Carcinogenesis References:

NCI TR-76 (1978); IARC (1979, 1987, 1999); *NTP Report on Carcinogens* (first listed in the second edition).

L736b; (cf. 2,3-isomer. in 192); 66/8; Not TSCA

RN 28700-28-9 REGISTRY

CN 1-Propanol, dibromo-, phosphate (3:1) (8CI, 9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

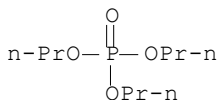
CN 1-Propanol, dibromo-, phosphate (6CI, 7CI)

OTHER NAMES:

CN Dibromopropyl phosphate

CN LV-T23P

CN **Tris(dibromopropyl) phosphate**



6 (D1-Br)

Search Statement and Results for L736b:

=> S TRIS(W)DIBROMOPROPYL(W)PHOSPHATE OR 28700-28-9

L24 10 TRIS(W) DIBROMOPROPYL(W) PHOSPHATE OR 28700-28-9

=> S LV(W)T23P

L25 0 LV(W) T23P

This CAS RN was probably assigned to tris(2,3-dibromopropyl) phosphate (L736; 126-72-7) when authors did not specify the location of the bromine atoms.

No records were retrieved in TOXLINE by use of the CAS RN.

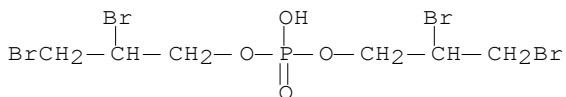
L737; 173, 192; 35/-; TSCA

RN 5412-25-9 REGISTRY

CN 1-Propanol, 2,3-dibromo-, hydrogen phosphate (8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN Bis(2,3-dibromopropyl) hydrogen phosphate

CN **Bis(2,3-dibromopropyl) phosphate***Search Statements and Results for L737:*

=> S BIS(2A)L1(2A)PHOSPHATE OR 5412-25-9

L26 154 BIS(2A) L1(2A) PHOSPHATE OR 5412-25-9

=> DUP REM L26

PROCESSING COMPLETED FOR L26

L27 35 DUP REM L26 (119 DUPLICATES REMOVED)

ANSWERS '1-17' FROM FILE MEDLINE

ANSWERS '18-19' FROM FILE CANCERLIT

ANSWER '20' FROM FILE AGRICOLA

ANSWERS '21-22' FROM FILE NIOSHTIC

ANSWERS '23-24' FROM FILE EMBASE

ANSWERS '25-26' FROM FILE BIOSIS

ANSWERS '27-34' FROM FILE TOXCENTER

ANSWER '35' FROM FILE LIFESCI

The CAS RN alone in EMIC retrieved eight records. Allowing TOXLINE to add synonyms retrieved 29 records. Combination of 126-72-7 (for the tris form) and bis retrieved 50 records in TOXLINE, and combination of 126-72-7 and metab* retrieved 99 records.

References:

Chem Service Inc., a supplier of analytical standards, was the only U.S. supplier listed in the CHEMCATS database for L737. Chem Service Inc. (1998) offered neat L737 in 5-g quantities.

IPCS (1997) listed L737 as a flame retardant for polypropylene. Use in children's clothing was banned in 1977 (IPCS, 1997).

As mentioned above, IPCS (1995b) (EHC No. 173) reviewed literature on L737 as a metabolite of L736, and this summary for L737 will mention only studies not cited by IPCS. (Published abstracts are excluded from the discussion.)

Elliott et al. (1983) reported that age-matched female rats were less sensitive to the nephrotoxicity of L737 than male rats. Cobaltous chloride pretreatment reduced the nephrotoxicity in males. The IARC (1999) evaluation of L736 included carcinogenesis studies of L737 magnesium salt (L737-Mg) and of L730 and mentioned that L737 was nephrotoxic. The TOXLINE record of an article by Koob and Dekant (1991), "Bioactivation of xenobiotics by formation of toxic glutathione conjugates," had no abstract but indexed the CAS RN of L737. Minegishi et al. (1988) compared ADME of several brominated and chlorinated phosphate flame retardants, including L737, in rats. Momma et al. (1982) (Japanese) studied the "Effect of oral administration of [L737] to pregnant rats on prenatal and postnatal developments [sic]." RTECS listed mammalian and bacteria genotoxicity tests. Sai et al. (1989) detected "8-hydroxydeoxyguanosine [a marker of oxidative DNA damage] in rat kidneys treated with renal carcinogens." The TOXLINE record had no abstract, but L737 was indexed. Tobe et al. (1985) (Japanese; no abstract) studied toxic renal injuries in rats induced by L737 and puromycin aminonucleoside and correlated urinary enzyme activities and histological changes.

L737-ALLYL; (cf. L738c); 6/3; Not TSCA

RN 33528-42-6 REGISTRY

CN Phosphoric acid, bis(2,3-dibromopropyl) 2-propenyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

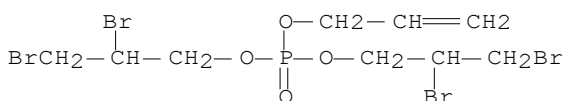
CN 1-Propanol, 2,3-dibromo-, allyl phosphate (2:1)

CN Phosphoric acid, allyl bis(2,3-dibromopropyl) ester (6CI, 8CI)

OTHER NAMES:

CN **Allyl bis(2,3-dibromopropyl) phosphate**

CN Bis(2,3-dibromopropyl) 2-propenyl phosphate

**L737-NH4; 192; 13/-; Not TSCA**

RN 34432-82-1 REGISTRY

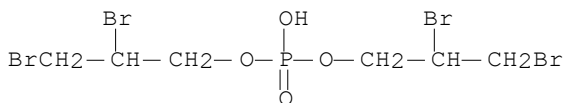
CN 1-Propanol, 2,3-dibromo-, hydrogen phosphate, ammonium salt (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Phosphoric acid, bis(2,3-dibromopropyl) ester, ammonium salt (8CI)

OTHER NAMES:

CN Ammonium bis(2,3-dibromopropyl) phosphate

CN **Bis(2,3-dibromopropyl) ammonium phosphate***Search Statement for L737-NH4:*

=> S BIS(6A)L1(6A)AMMONIUM OR 34432-82-1

L28 7 BIS(6A) L1(6A) AMMONIUM OR 34432-82-1

=> DUP REM L28

PROCESSING COMPLETED FOR L28

L29 5 DUP REM L28 (2 DUPLICATES REMOVED)

ANSWER '1' FROM FILE BIOTECHNO

ANSWERS '2-5' FROM FILE TOXCENTER

[Has RTECS record.] Use of the CAS RN in EMIC retrieved three records.

References:

IPCS (1997) listed this salt as a flame retardant. When Aoyama (1975a) exposed mice to fumes from burning clothing containing L737-NH4 as the flame retardant, their deaths were due to carbon monoxide poisoning. The skin of rats and rabbits was irritated by aqueous solutions of L737-NH4 tested in concentrations up to 30% (Aoyama, 1975b). L737-NH4 was a strong inhibitor of acid phosphatase in the skin of guinea pigs; it also inhibited skin cholinesterase (Fujise et al., 1984). Ikeda et al. (1985) included this compound in studies of acute oral and cutaneous toxicities of ten chemicals found in household goods. The RTECS record listed Salmonella test data from Nakamura et al. (1983; cited in IPCS, 1995b).

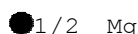
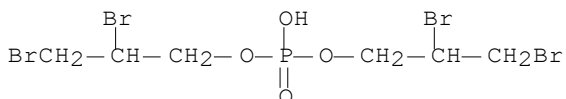
L737-Mg; 192; 1/-; Not TSCA

RN 36711-31-6 REGISTRY

CN 1-Propanol, 2,3-dibromo-, hydrogen phosphate, magnesium salt (9CI) (CA INDEX NAME)

OTHER NAMES:

CN DB 1

CN **Magnesium bis(2,3-dibromopropyl) phosphate***Search Statement and Results for L737-Mg:*

=> S 36711-31-6 OR L1(6A)PHOSPHATE(6A)MAGNESIUM

L30 22 36711-31-6 OR L1(6A) PHOSPHATE(6A) MAGNESIUM

=> DUP REM L30

L31 6 DUP REM L30 (16 DUPLICATES REMOVED)

ANSWERS '1-2' FROM FILE MEDLINE

ANSWER '3' FROM FILE BIOTECHNO

ANSWER '4' FROM FILE EMBASE

ANSWER '5' FROM FILE BIOSIS

ANSWER '6' FROM FILE LIFESCI

[Has RTECS record.]

References:

IPCS (1997) listed this salt as a flame retardant. The RTECS record lists a mutation test in Salmonella, a reproductive toxicity study in rats, a 45-day oral study in rats, and an acute oral toxicity study in rats. Included in IPCS (1995b): Takada et al. (1996) fed male and female Wistar rats L737-Mg in the diet at concentrations up to 2000 ppm for 24 months, inducing hepatocellular carcinomas in males and other tumors in both sexes. [See also CCRIS (1992) and IARC (1999).] Nakamura et al. (1979, 1983) tested L737-Mg in Salmonella tester strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538.

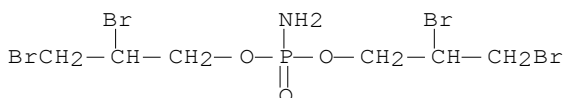
L737-PONH2; -, 2/-; Not TSCA

RN 70555-34-9 REGISTRY

CN Phosphoramidic acid, bis(2,3-dibromopropyl) ester (9CI) (CA INDEX NAME)

OTHER NAMES:

CN DB 2

CN **Bis(2,3-dibromopropyl) phosphoramidate***Reference:*

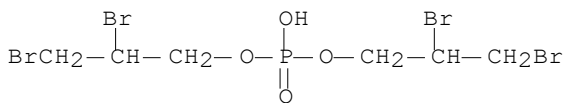
Salmonella testing by Nakamura et al.(1979; cited in IPCS, 1995b) is listed for L730-PONH2 in RTECS. Testing was also reported by Nakamura et al. (1983; cited in IPCS, 1995b).

L737-K; 192; 1/-; Not TSCA

RN 66519-18-4 REGISTRY

CN 1-Propanol, 2,3-dibromo-, hydrogen phosphate, potassium salt (9CI) (CA INDEX NAME)

CN **Potassium bis(2,3-dibromopropyl) phosphate**



Search Statement and Results for L737-K:

=> S 66519-18-4 OR L1(6A)PHOSPHATE(6A)POTASSIUM
L32 0 66519-18-4 OR L1(6A) PHOSPHATE(6A) POTASSIUM

References:

IPCS (1997) listed this salt as a flame retardant.

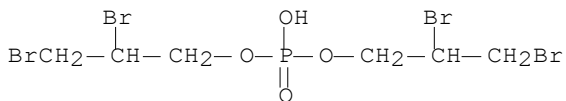
L737-Na; 192; 2/-; Not TSCA

RN 64864-08-0 REGISTRY

CN 1-Propanol, 2,3-dibromo-, hydrogen phosphate, sodium salt (9CI) (CA INDEX NAME)

OTHER NAMES:

CN **Sodium bis(2,3-dibromopropyl) phosphate**



Search Statement and Results for L737-Na:

=> S 64864-08-0
L33 0 64864-08-0

=> S L1(6A)PHOSPHATE(6A)SODIUM
L34 3 L1(6A) PHOSPHATE(6A) SODIUM

=> DUP REM L34
PROCESSING COMPLETED FOR L34
L35 1 DUP REM L34 (2 DUPLICATES REMOVED)
ANSWER '1' FROM FILE NIOSHTIC

[Has RTECS record.]

References:

IPCS (1997) listed this salt as a flame retardant. The RTECS record lists only a Salmonella test reported in 1982.

L737-mono; 192; 18/1; Not TSCA

RN 5324-12-9 REGISTRY

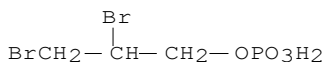
CN 1-Propanol, 2,3-dibromo-, dihydrogen phosphate (6CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2,3-Dibromopropyl dihydrogen phosphate

CN **Mono(2,3-dibromopropyl) phosphate**

CN Phosphoric acid mono(2,3-dibromopropyl) ester

*Search Statement and Results for L737-mono:*

=> S 51258-03-8 OR 2(W)3(W)DIBROMO(W)1(W)PROPANOL(W)PHOSPHATE

L36 8 51258-03-8 OR 2(W) 3(W) DIBROMO(W) 1(W) PROPANOL(W) PHOSPHATE

=> DUP REM L36

L37 1 DUP REM L36 (7 DUPLICATES REMOVED)

ANSWER '1' FROM FILE MEDLINE

[Later found the more appropriate CAS RN.] No results were found in TOXLINE for the CAS RN listed above.

References:

2,3-Dibromo-1-propanol phosphate was listed in IPCS (1997) as a flame retardant for which ITC had deferred testing. Holme et al. (1983; cited by IPCS, 1985b) tested L737-mono in several genotoxicity assays. An article by Shirai et al. (1984) was entitled "Promotion of 2-(ethylnitrosoamino)ethanol-induced renal carcinogenesis in rats by nephrotoxic compounds: Positive responses with folic acid, basic lead acetate, and *N*-(3,5-dichlorophenyl)succinimide but not with 2,3-dibromo-1-propanol phosphate," but the latter meant the tris compound (L736) not the monoester. "Tris-BP" followed the name in the abstract, yet the TOXLINE record was indexed with the CAS RN of the monoester. Söderlund et al. (1982 lett.; cited by IPCS, 1995b) reported on the mutagenicity and nephrotoxicity of L737-mono as well as L736 and L737.

L737-mono-NH4; -; 2/-; Not TSCA

RN 63262-57-7 REGISTRY

CN 1-Propanol, 2,3-dibromo-, dihydrogen phosphate, monoammonium salt (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Ammonium 2,3-dibromopropyl phosphate

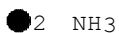
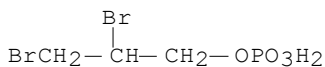
*References:*

Ikeda et al. (1985) included this compound in studies of acute oral and cutaneous toxicities of ten chemicals found in household goods. Nakamura et al. (1983; cited by IPCS, 1995b) tested this compound in Salmonella.

L737-mono-2NH4; -; 1/-; Not TSCA

RN 85771-01-3 REGISTRY

CN 1-Propanol, 2,3-dibromo-, dihydrogen phosphate, diammonium salt (9CI) (CA INDEX NAME)

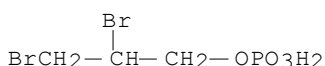
*Reference:*

RTECS lists a Salmonella test reported in *Mutation Research* in 1983 (Nakamura et al., 1983; cited by IPCS, 1995b).

L737-mono-Mg; -; 2/-; Not TSCA

RN 43110-33-4 REGISTRY

CN 1-Propanol, 2,3-dibromo-, dihydrogen phosphate, magnesium salt (1:1) (9CI) (CA INDEX NAME)

*References:*

Nakamura et al. (1983; cited by IPCS, 1995b) tested this compound in Salmonella.

L738a; 192; 9/-; Not TSCA

RN 21661-76-7 REGISTRY

CN Phosphonic acid, bis(2,3-dibromopropyl) ester (8CI, 9CI) (CA INDEX NAME)

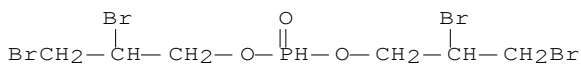
OTHER CA INDEX NAMES:

CN 1-Propanol, 2,3-dibromo-, phosphonate (2:1)

OTHER NAMES:

CN **Bis(2,3-dibromopropyl) phosphite**

CN Di(2,3-dibromopropyl) phosphite

*Search Statement and Results for L738a:*

=> S 21661-76-7 OR (BIS OR DI)(W)L1(W)(PHOSPHITE OR PHOSPHONATE)

L38 1 21661-76-7 OR (BIS OR DI)(W) L1(W)(PHOSPHITE OR PHOSPHONATE)

=> DUP REM L38

PROCESSING COMPLETED FOR L38

L39 1 DUP REM L38 (0 DUPLICATES REMOVED)

ANSWER '1' FROM FILE TOXCENTER

No records were retrieved in TOXLINE for the CAS RN.

References:

IPCS (1997) listed L738a as a flame retardant for which testing by ITC had been deferred. No CAS RN was identified for the unspecific isomer listed in IPCS (1997) that would have been **L738b**.

L738c; 192; 3/1; Not TSCA

RN 10519-68-3 REGISTRY

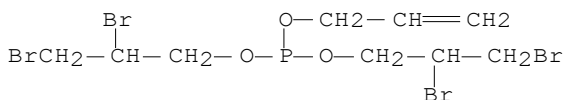
CN Phosphorous acid, allyl bis(2,3-dibromopropyl) ester (7CI, 8CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1-Propanol, 2,3-dibromo-, allyl phosphite (2:1) (8CI)

OTHER NAMES:

CN **Allyl bis(2,3-dibromopropyl) phosphite**

*Search Statements and Results for L738c:*

=> S ALLYL(6A)L1

L40 0 ALLYL(6A) L1

=> S ALLYL?(6A)L1

L41 0 ALLYL?(6A) L1

=> S 10519-68-3

L42 0 10519-68-3

References:

IPCS (1997) listed L738c as a flame retardant for which ITC had deferred testing.

L739c; 192 (nonspecific); 4/1; Not TSCA

RN 55190-46-0 REGISTRY

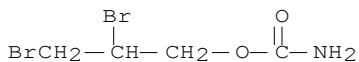
CN 1-Propanol, 2,3-dibromo-, carbamate (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Carbamic acid, 2,3-dibromopropyl ester (6CI)

OTHER NAMES:

CN **2,3-Dibromopropyl carbamate**

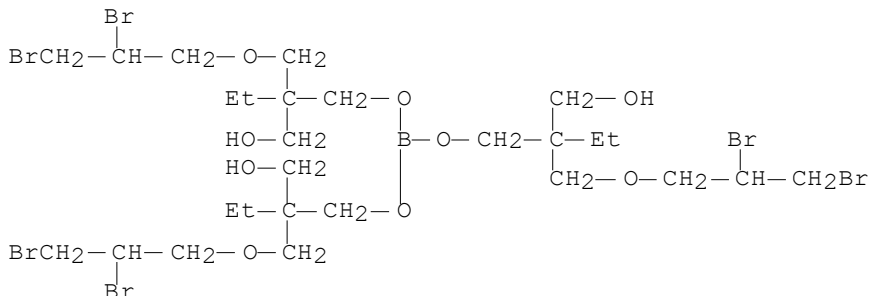
*References:*

Chem Service (1998) supplied neat dibromopropyl carbamate in 10-g quantities. Both “dibromopropyl carbamate” and “bis(dibromopropyl) carbamate” were listed in IPCS (1997) among compounds for which ITC had deferred testing. No other information was found for the latter compound, which could not be identified in the Registry file.

Uncoded TSCA-Listed Compounds That Had No Database Records

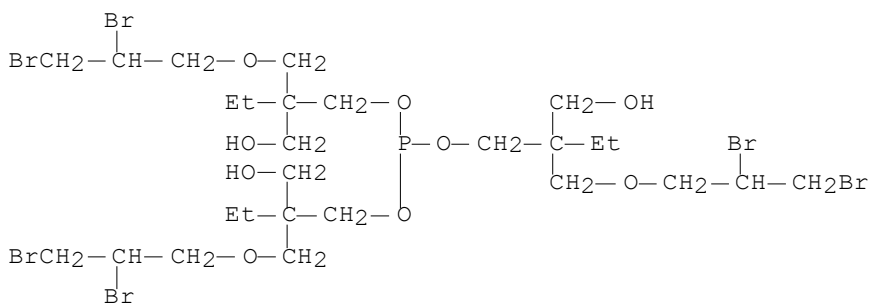
RN 68555-83-9 REGISTRY

CN 1,3-Propanediol, 2-[(2,3-dibromopropoxy)methyl]-2-ethyl-, ester with boric acid (H3BO3) (3:1) (9CI) (CA INDEX NAME)



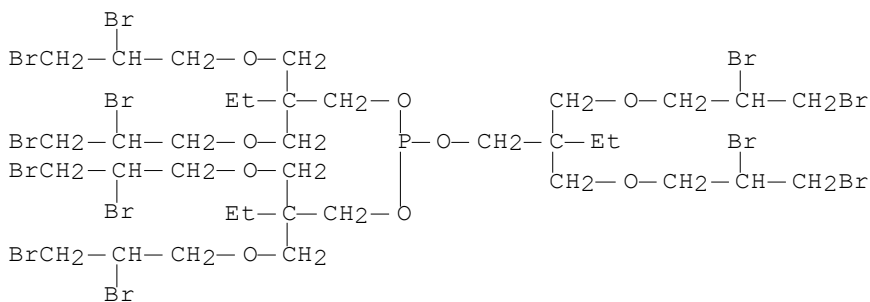
RN 68555-84-0 REGISTRY

CN 1,3-Propanediol, 2-[(2,3-dibromopropoxy)methyl]-2-ethyl-, phosphite (3:1) (9CI) (CA INDEX NAME)

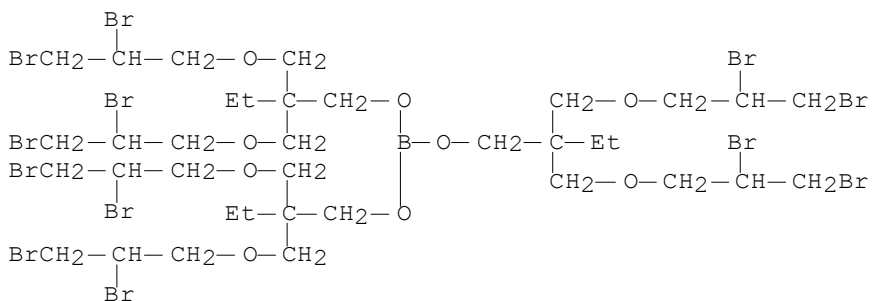


RN 68555-85-1 REGISTRY

CN 1-Butanol, 2,2-bis[(2,3-dibromopropoxy)methyl]-, phosphite (3:1) (9CI) (CA INDEX NAME)



RN 68555-87-3 REGISTRY

CN 1-Butanol, 2,2-bis[(2,3-dibromopropoxy)methyl]-, triester with boric acid (H3BO3) (9CI)
(CA INDEX NAME)

RN 68647-21-2 REGISTRY

CN Boric acid, 2,2-bis[(2,3-dibromopropoxy)methyl]butyl ester (9CI) (CA INDEX NAME)

MF C12 H22 Br4 O3 . x Unspecified

LC STN Files: CHEMLIST

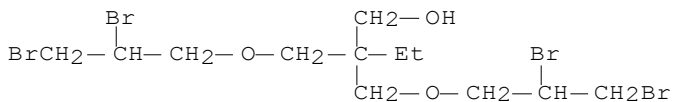
Other Sources: NDSL**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

CM 1

CRN 224620-17-1

CMF C12 H22 Br4 O3



CM 2

CRN 11113-50-1

CMF Unspecified

CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***