TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVP SUBSTANCES

RESULTS OF THE EVALUATION OF THE PBT/VPVB PROPERTIES OF:

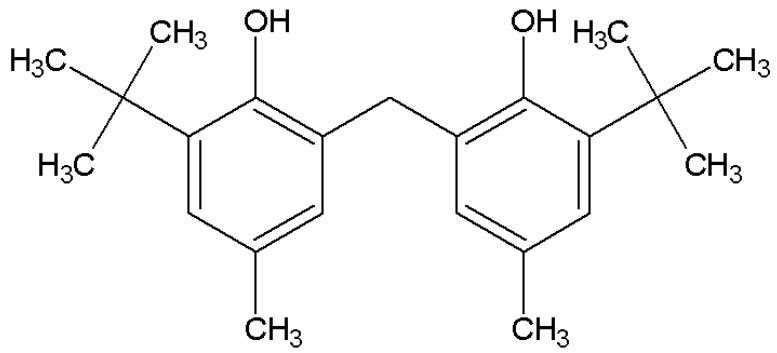
Substance name: 6,6'-Di-tert-butyl-2,2'-methylenedi-p-cresol

EC number: 204-327-1

CAS number: 119-47-1

Molecular formula: $C_{23}H_{32}O_2$

Structural formula:



Summary of the evaluation:

The substance is not considered to be a PBT substance. It does not meet the B or T criteria. It does meet the screening criteria for P (and vP).

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: 6,6'-Di-tert-butyl-2,2'-methylenedi-p-cresol
EC Number: 204-327-1
CAS Number: 119-47-1
IUPAC Name:
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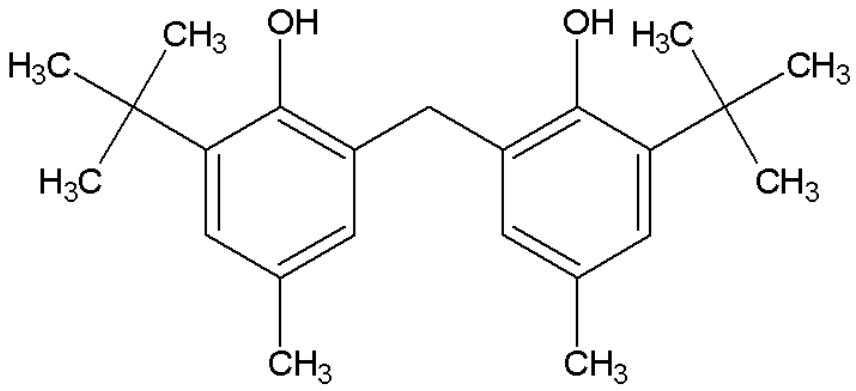

Molecular Weight: 340.51 g/mole
Synonyms: 2,2’-Methylene-bis(4-methyl-6-tert-butyl phenol);

2,2’-Methylene-bis(6,6’-tert-butyl-p-cresol);

2,2’-Methylene-bis(6-tert-butyl-4-methylphenol);

2,2’-Dihydroxy-3,3’-di-tert-butyl-5,5’-dimethyldiphenylmethane;

Bis-(2-hydroxy-3-tert-butyl-5-methylphenyl)methane;

Bis-(6-hydroxy-3-methyl-5-tert-butylphenyl)methane;

p-Cresol, 2,2’-methylene-bis(6-tert-butyl);

Phenol, 2,2’-methylene-bis(6-(1,1-dimethylethyl)-4-methyl);

The abbreviation DBMC will be used in this assessment.

1.1 Purity/Impurities/Additives

The purity of DBMC is reported to be ≥98.0% by weight. No additives are reported to be present in the commercial substance (OECD, 2000).

1.2 Physico-Chemical properties

Table 1 Summary of physico-chemical properties

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 KPa	solid (supplied as a pale cream to white powder or granules)	
V, 5.2	Melting / freezing point	130°C	
V, 5.3	Boiling point	445°C	Estimation by MPBPWIN (v1.41)
V, 5.5	Vapour pressure	4.6×10-7 Pa at 20°C	Estimation (Environment Agency, 2008)
V, 5.7	Water solubility	0.92 mg/l at 20°C[a]	Column elution method
V, 5.8	Partition coefficient n-octanol/water (log value)	6.25 at 20°C	Shake flask method
VII, 5.19	Dissociation constant	≥10	The pKa values of o , m- and p-cresol are 10.2, 10.01 and 10.17, respectively (CRC, 1979). Therefore the pKa value of the DBMC is likely to be around 10 and above.

[a] A European supplier has provided details of a water solubility determination by the column elution method (Lanxess, personal communication, 2005). This study was carried out in 1989, but was not reported in OECD (2000). Although some details are lacking, the method appears to comply with the OECD Test Guideline (107). Determinations were carried out at 20°C at two different flow rates, which gave results in good agreement (0.88 and 0.96 mg/L). The mean solubility value was 0.92 mg/L. The test substance concentration was determined by HPLC analysis, and this showed only one peak. It is therefore unlikely that the result was influenced by soluble impurities. The column elution method is appropriate for substances of low solubility (10 mg/L or less). Since no details appear to be available about the method used for the test cited by OECD (2000), the solubility of 0.92 mg/L is preferred.

2 MANUFACTURE AND USES

Not relevant.

3 CLASSIFICATION AND LABELLING

DBMC is not currently classified as dangerous for the environment under the Dangerous Substances Directive (67/548/EEC). DBMC is not readily biodegradable. It has a measured BCF of 840. The lowest acute value reported is L(E)C50 = 0.31 mg/l. On the basis of these values, the indicated classification is "Dangerous for the environment" with the risk phrases R50-53: very toxic to aquatic organisms and may cause long-term adverse effects in the aquatic environment

3.1 Degradation (P)

3.1.1 Abiotic degradation

Hydrolysis

DBMC does not contain functional groups that are susceptible to hydrolysis in the environment. Hydrolysis is therefore not expected to be a significant degradation process in the environment.

Oxidation

There are no data on the reactions of DBMC with oxidants present in water. DBMC would be expected to react reasonably rapidly with hydroxyl radicals in freshwater resulting in primary degradation.

3.2 Biotic degradation

The biodegradation data for DBMC have been reviewed as part of the OECD SIDS programme (OECD, 2000). The substance has been tested in a MITI I (equivalent to OECD 301C) ready biodegradation test (CITI, 1992; CERI, 2004). The concentration of the test substance used was 100 mg/l and the inoculum concentration was 30 mg/l as suspended solid. The source of the inoculum was non-adapted activated sludge. The extent of degradation seen after 28 days was 0% based on oxygen consumption. The lack of degradation in the study was confirmed by analysis for the parent compound by HPLC. This analysis showed that only around 1% of the substance had been removed over the 28-day period.

Based on the results of this test DBMC is considered to be not readily biodegradable. It should be noted however that the concentration tested was in excess of the water solubility of DBMC (0.92 mg/l). This may have limited the availability of the DBMC to the micro-organisms in the test.

3.2.1 Other information [1]

3.2.2 Summary and discussion of persistence

The results of biodegradation tests indicate that the substance is not readily biodegradable.

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[1] For example, half life from field studies or monitoring data

3.3 Environmental distribution

3.3.1 Adsorption

3.3.2 Volatilisation

3.4 Bioaccumulation (B)

3.4.1 Screening data[2]

3.4.2 Measured bioaccumulation data[3]

The available bioconcentration study for DBMC has been reviewed under the OECD SIDS programme (OECD, 2000). The study was an eight week flow-through study using carp (Cyprinus carpio) with an average lipid content of 4.7% (CITI, 1992; CERI, 2004). Two exposure concentrations were used, 1.0 mg/l and 0.1 mg/l, and it was reported that the stock solutions of the test substance were prepared with caster oil HCO-40, which would have then been present in the exposure vessels. The exposure concentrations were verified by analytical measurement during the test and were found to be maintained within 80% of the nominal values throughout the test. The BCF value obtained was 23-37 l/kg at the 1.0 mg/l exposure level and 60-125 l/kg at the 0.1 mg/l exposure level.

It should be noted that the BCF values obtained appeared to decrease with increasing exposure concentration. This pattern may occur where solubility of the test substance has been exceeded and undissolved test substance is present. It is not clear if the analytical method used would distinguish between the dissolved test substance and the total test substance present. The higher concentration used in the test was slightly above the solubility value of 0.92 mg/l used in this assessment (both concentrations were above the value of 0.02 mg/l selected in the OECD SIDS). Further, OECD (2000) recognises that there is the possibility that the substance could have adsorbed to the skin of the fish during the study and/or have adsorbed to the food during the study (and so providing an oral route of exposure for the fish). Therefore the results of this test should be treated with caution.

From experience with other BCF studies reported from the same source, the range of values presented is likely to relate to the lowest and highest BCF values measured in individual fish from the tests. The mean values for each concentration would be the more relevant values, but in the absence of these the highest reported value would be used as a conservative approach.

The Japanese National Institute of Technology and Evaluation (NITE) web-site includes other data on bioaccumulation from tests carried out in Japan. These tests used concentrations of 2.0 and 0.2 µg/l in 60-day tests with carp. Few other details are included, but the tests are assumed to be carried out using the standard methods and so are comparable with those discussed above. The BCF values obtained were 400-840 at 2.0 µg/l, and 320-780 at 0.2 µg/l. The test concentrations are well below

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2 For example, log K_{ow} values, predicted BCFs

3 For example, fish bioconcentration factor

the solubility values, and these results are considered to be the most suitable for use in the assessment. As noted above, the range of values is likely to relate to individual determinations in the tests, but in the absence of mean values the highest value will be used. Therefore the BCF used in this assessment is 840.

3.4.3 Other supporting information[4]

3.4.4 Summary and discussion of bioaccumulation

The measured BCF value in fish is 840.

3.5 Secondary poisoning

4 HUMAN HEALTH HAZARD ASSESSMENT

The mammalian and avian toxicity for DBMC have been reviewed as part of the OECD SIDS programme and a summary of the main findings of this review is given below in Table 2.

Table 2 Summary of mammalian toxicity data

Test	Species	Results
Acute oral (single dose) studies	Rat	>5,000 mg/kg be
Repeated dose studies – oral exposure	Rat	53 day NOAEL = 12.5 mg/kg bw day (males testis)
Developmental toxicity/ teratogenicity	Rat	Preliminary reproduction study –NOAEL = 50 mg/kg bw day (females)

[4]For example, measured concentrations in biota

5 ENVIRONMENTAL HAZARD ASSESSMENT

5.1 Aquatic compartment (including sediment)

5.1.1 Toxicity test results

5.1.1.1 Fish

Acute toxicity

The available toxicity data for DBMC have been reviewed and validated under the OECD SIDS programme (OECD, 2000). The following values were reported: 48h-LC50 >500 mg/l, 96h-LC50 >5 mg/l for medaka (Oryzias latipes) and 96h-LC50 = 0.31 mg/l for fathead minnow (Pimephales promelas). It was recognised that there was some uncertainty connected with these toxicity values as they were all considerably above the water solubility of the test substance. The OECD SIDS data set (OECD, 2000) contains a further toxicity result for DBMC with fish. The 48h-LC50 with orfe (Leuciscus idus) was reported to be 50 mg/l but there is insufficient information available to validate the study. Great Lakes (2004a) report further unpublished LC50 values for DBMC. The LC50 (duration not given) with orfe (Leuciscus idus) is reported as >100 mg/l and the 96h-LC50 for fish (species not given) is reported as >50 mg/l. Again few other details of these studies are currently available.

In the light of the revised water solubility used for this assessment (0.92 mg/l at 20°C, study made available since the OECD SIDS assessment), the LC50 value of 0.31 mg/l is now below the solubility and considered reliable.

Long-term toxicity

No data available.

5.1.1.2 Aquatic invertebrates

Acute toxicity

The available toxicity data for DBMC have been reviewed and validated under the OECD SIDS programme (OECD, 2000). The 48h-EC50 for Daphnia magna was determined to be >4.8 mg/l. It was recognised that there was some uncertainty connected with this toxicity value as it was above the water solubility of the test substance.

Long-term toxicity

The available toxicity data for DBMC have been reviewed and validated under the OECD SIDS programme (OECD, 2000). A 21-day NOEC of 0.34 mg/l was reported for DBMC in a Daphnia magna reproduction study. The OECD assessment recognised that there was some uncertainty connected with this toxicity value as it was considerably above the water solubility of the test

substance; however, the value is below the preferred solubility value used in this assessment (0.92 mg/l at 20°C, study made available since the OECD SIDS assessment) and so the result is considered to be suitable for this assessment.

5.1.1.3 Algae and aquatic plants

The available toxicity data for DBMC have been reviewed and validated under the OECD SIDS programme (OECD, 2000). A 72h-EC50 of >5 mg/l was reported for DBMC for the green alga Selenastrum capricornutum (now Pseudokirchneriella subcapitata) based on both biomass and growth rate endpoints. The 72h NOEC from this study was 0.63 mg/l based on biomass and 1.3 mg/l based on growth rate. These values are close to or above the solubility of the substance selected for this assessment.

5.1.2 Sediment organisms

5.1.3 Other aquatic organisms

5.2 Terrestrial compartment

5.3 Atmospheric compartment

5.4 Indirect exposure via the food chain

6 PBT AND vPvB

6.1 PBT, vPvB assessment

Persistence: the substance is considered to be not readily biodegradable so the screening criterion for P/ vP is met.

Bioaccumulation: a reliable *in vivo* experimental bioconcentration factor (BCF) of 840 has been measured for fish. Hence the substance does not meet the B (or vB) criterion.

Toxicity: The lowest LC50 is 0.31 mg/L for fish and the lowest NOEC = 0.34 mg/L for Daphnia. The T criterion is not met, although a full dataset is not available.

Summary: DBMC does not meet the T, B or vB criteria, and so is not considered a PBT substance according to the EU criteria.

INFORMATION ON USE AND EXPOSURE

Not relevant as substance is not identified as a PBT.

OTHER INFORMATION

The information used in this report was taken from the following sources:

CERI (2004). Biodegradation and bioaccumulation data of existing chemicals. Chemicals Evaluation and Research Institute Website http://www.cerij.or.jp/ceri_en/index_e4.shtml.

CITI (1992). Biodegradation and bioaccumulation data of existing chemicals based on the CSCL Japan. Chemicals Inspection and Testing Institute of Japan, as reported in OECD (2000).

CRC (1979). CRC Handbook of chemistry and physics. 60th Edition. CRC Press.

Environmental Risk Evaluation Report: 6,6'-Di-tert-butyl-2,2'-methylene-di-p-cresol (DBMC) CAS no. 119-47-1. Environment Agency of England and Wales, 2008 (to be published).

Great Lakes (2004a). Technical Information and Material Safety Data Sheet for Lowinox 22M46. Great Lakes Polymer Additives. http://www.pa.greatlakes.com.

OECD (2000). OECD SIDS Dossier for 6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol, CAS No. 119-47-1.