TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

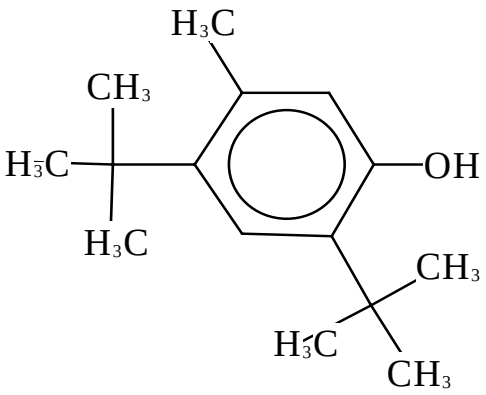
Substance name: 4,6-di-tert-butyl-m-cresol

EC number: 207-847-7

CAS number: 497-39-2

Molecular formula: C15H24O

Structural formula:



Summary of the evaluation:

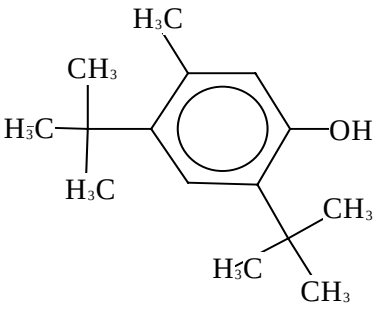
4,6-di-tert-butyl-m-cresol is not considered to be a PBT substance. This conclusion concerns only the parent compound.

The substance does not meet the B criterion. It may meet the P/vP criteria based on screening data. Although 4,6-di-tert-butyl-m-cresol may degrade according to the data on the isomer BHT (2,6-di-tert-butyl-m-cresol; CAS 128-37-0), no estimate on the rate of degradation is available. The assessment of ecotoxicity was not completed. The conclusion is mainly based on the data available on the isomer BHT (PBT Summary fact sheet No. 121).

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: 4,6-di-tert-butyl-m-cresol
EC Number: 207-847-7
CAS Number: 497-39-2
IUPAC Name:
Molecular Formula: C15H24O
Structural Formula:



Molecular Weight: 220.35
Synonyms: Di-tert.-butyl-m-kresol; phenol, 2,4-bis(1,1-dimethylethyl)-5-methyl-

1.1 PURITY/IMPURITIES/ADDITIVES

No data available.

1.2 PHYSICO-CHEMICAL PROPERTIES

Table 1 Summary of physico-chemical properties. For details and references, see European Commission (2000).

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 Kpa	solid	European Commission (2000)
V, 5.2	Melting/freezing point	62.1ºC	Beilstein E III 6, 2072 (data not evaluated)
V, 5.3	Boiling point	282ºC (at 1013 hPa)	Beilstein E III 6, 2072 (data not evaluated)
V, 5.5	Vapour pressure	13 hPa (at 150ºC) 130 hPa (at 244ºC)	Beilstein E III 6, 2072 (data not evaluated)
V, 5.7	Water solubility	8.2 mg l^{-1} (at 20ºC)	Bayer AG data (data not evaluated)
V, 5.8	Partition coefficient n-octanol/water (log value)	5.04 (at 21ºC) 5.88	Bayer AG data (data not evaluated) Calculated (KOWWIN v1.67)
VII, 5.19	Dissociation constant	8-11	For hydroxylated aryl compounds (Rochester, 1971) (data not evaluated)

2 MANUFACTURE AND USES

One company has provided information on the substance under Regulation 93/793/EEC. The substance is according to industry used solely as an on-site intermediate and it is not on the market.

3 CLASSIFICATION AND LABELLING

The substance is not classified in the Annex I of Directive 67/548/EEC.

4 ENVIRONMENTAL FATE PROPERTIES

4.1 DEGRADATION (P)

4.1.1 Abiotic degradation

For this substance, no experimental data are available regarding abiotic degradation. The isomer 2,6-di-tert-butyl-m-cresol (BHT, CAS 128-37-0) is known to form oxidation products in aquatic solutions both with and without UV-radiation (see PBT Summary fact sheet No. 121).

Indirect photochemical degradation in the atmosphere is considered to be fast based on the estimated half-life of 3.04 h for the reaction with OH radicals with AOP v1.91 (24 h day^{-1}; $5 \cdot 10^5$ OH^- cm^{-3}).

4.1.2 Biotic degradation

4,6-di-tert-butyl-m-cresol degraded 0% in 28 days in a ready biodegradability test according to Directive 84/449/EEC C.7 (modified MITI; Bayer AG data). It is noted that the study report was not available to the Rapporteur and the result was therefore not evaluated.

The isomer 2,6-di-tert-butyl-m-cresol (BHT) was degraded very little (4.5%) in a modified MITI test (MITI 1992). In addition, BHT was observed to be degraded in three soils both via abiotic and biological processes (see PBT Summary fact sheet No. 121).

4.1.3 Other information [1]

No data available.

4.1.4 Summary and discussion of persistence

4,6-di-tert-butyl-m-cresol is not readily biodegradable according to a standard modified MITI-test. However, reading across from the data on the isomer 2,6-di-tert-butyl-m-cresol (BHT; CAS 128-37-0), 4,6-di-tert-butyl-m-cresol is expected to oxidise in water in a moderate to rapid rate forming various reaction products. The aquatic studies available on the isomer BHT do not provide information on the rate and type of further degradation. Degradation in sediment may deviate considerably from the degradation in water due to different redox- conditions. Degradation in soil can be expected to occur, but the rate of degradation in environmentally relevant conditions is not

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

known. Further testing of degradation is necessary to complete the assessment of persistency. As a first step, testing of the isomer BHT should be approached. Further testing needs of BHT have been specified in the PBT Summary fact sheet No. 121.

4.2 ENVIRONMENTAL DISTRIBUTION

Data not reviewed for this report.

4.2.1 Adsorption

4.2.2 Volatilisation

4.2.3 Long-range environmental transport

4.3 BIOACCUMULATION (B)

4.3.1 Screening data[2]

Using the measured logKow of 5.04, a BCF of 538 was derived by BCFWIN v2.15. With the estimated logKow –value of 5.88 a BCF of 2,382 results. The equation used in the TGD provides a BCF of 3,837 with logKow of 5.04. It is noted, that BCFWIN identifies the substance as tert-butyl ortho-phenol type calculating a correction factor for this species, whereas the TGD –model only accounts for the logKow. It is noted, that for the isomer BHT a measured logKow of 5.1 and estimated logKow values of 5.03 - 6.2 are available (see PBT Summary No. 121).

4.3.2 Measured bioaccumulation data[3]

No measured data on bioaccumulation are available for 4,6-di-tert-butyl-m-cresol. For the isomer BHT (CAS 128-37-0) an experimental BCF (sampling occasion means 520-1,276; min-max of individual BCFs 220-2,800) has been derived by MITI (1992). For the references and details, see PBT Summary fact sheet No. 121.

4.3.3 Other supporting information[4]

No data available.

4.3.4 Summary and discussion of bioaccumulation

Reading across from the experimental BCF on the isomer BHT, it is concluded that 4,6-di-tert-butyl-m-cresol has a moderate to high bioaccumulation potential, but the BCF is expected to remain below 2,000. The BCF predicted based on the experimental logKow –value supports the conclusion.

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

3 For example, fish bioconcentration factor

4For example, measured concentrations in biota

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

According to Bayer AG data, a LC_{50}(96h) of 2.3 mg l^{-1} was obtained for *Brachydanio rerio* in a test according to "UBA-Verfahrensvorschlag, Lethale Wirkung beim Zebrabaerbling *Brachydanio rerio*, Mai 1984". Part of the test substance remained undissolved. It is noted that the study was not available to the Rapporteur for evaluation.

ECOSAR v0.99h allocates the substance to the category of phenols. A LC_{50} (96 hours) of 0.43 mg l^{-1} is estimated using the logKow of 5.04.

Long-term toxicity

No experimental data are available. DK-QSAR database provides a chronic NOEC of 0.006 mg l^{-1}. ECOSAR v0.99h predicts for fish a chronic NOEC (90 days) of 0.012 mg l^{-1}(logKow of 5.04 used).

6.1.1.2 Aquatic invertebrates

Acute toxicity

No experimental data are available. ECOSAR v0.99h estimates a LC_{50} (48 hours) of 0.68 mg l^{-1} using the logKow of 5.04.

Long-term toxicity

No experimental data are available for 4,6-di-tert-butyl-m-cresol. For the isomer BHT a 2 day-NOEC of 0.07 mg l^{-1} has been derived by Bayer AG (1994).

ECOSAR v0.99h predicts for daphnids a chronic NOEC of 0.05 mg l^{-1} (logKow of 5.04 used).

6.1.1.3 Algae and aquatic plants

No experimental data are available. ECOSAR v0.99h estimates an EC_{50} (96 hours) of 0.22 mg l^{-1} using logKow of 5.04. The NOEC estimate is 0.13 mg l^{-1}.

6.1.2 Sediment organisms

No data available.

6.1.3 Other aquatic organisms

In a test with activated sludge according to ISO 8192 ("Test for inhibition of oxygen consumption by activated sludge") a 3-hour EC_0 of 10,000 mg l^{-1} was determined (Bayer AG data).

6.2 TERRESTRIAL COMPARTMENT

No data available.

6.3 ATMOSPHERIC COMPARTMENT

No data available.

7 PBT AND VPVB

7.1 PBT, VPVB ASSESSMENT

Persistence: 4,6-di-tert-butyl-m-cresol may meet the P/vP criteria based on screening data. The substance is not readily biodegradable, but it is based on the data of the isomer 2,6-di-tert-butyl-m-cresol (BHT; CAS 128-37-0; PBT Summary No. 121) expected to oxidise in water to several transformation products. The environmentally relevant rate of degradation of the isomer BHT is not known. Degradation rate in sediment may deviate considerably from the degradation rate in water due to a different oxygen regime. 4,6-di-tert-butyl-m-cresol can be expected to degrade in soil but the rate of degradation cannot be estimated. Further testing on degradation would be needed, whereas the isomer BHT could be first targeted for testing. Especially soil and sediment tests are necessary to determine environmentally relevant rates of degradation. However, such testing is not required for the PBT-assessment due to the overall conclusion (see below).

Bioaccumulation: 4,6-di-tert-butyl-m-cresol does not meet the B criterion. The experimental BCF of the isomer BHT for fish is below 2,000. This conclusion applies for the parent compound, only.

Toxicity: No chronic ecotoxicity data are available for 4,6-di-tert-butyl-m-cresol. One chronic study is available for the isomer BHT (*Daphnia magna*, NOEC 0.07 mg l^{-1}). The QSAR predictions indicate that acute and chronic toxicity would be just above the triggers of 0.1 mg l^{-1} and 0.01 mg l^{-1} when using the experimental logKow (5.04). If the estimated logKow is applied, ecotoxicity criterion would seem to be fulfilled. Hence, 4,6-di-tert-butyl-m-cresol may fulfil the T criterion, but data on long-term effects are needed to complete the assessment. Further testing is, however, not required due to the overall conclusion (see below).

Summary: 4,6-di-tert-butyl-m-cresol substance does not meet the B criterion. It may meet the P/vP criteria based on screening data. Although 4,6-di-tert-butyl-m-cresol may degrade according to the data on the isomer BHT (2,6-di-tert-butyl-m-cresol; CAS 128-37-0), no estimate on the rate of degradation is available. The assessment of ecotoxicity was not completed. The PBT-assessment is mainly based on the data available on the isomer 2,6-di-tert-butyl-m-cresol (PBT Summary fact sheet No. 121).

It is concluded that the substance is not considered as a PBT substance. This conclusion concerns the parent compound only.

INFORMATION ON USE AND EXPOSURE

Not relevant as the substance is not identified as a PBT.

OTHER INFORMATION

The information and references used in this report were taken from the following source:

European Commission (2000) IUCLID Dataset, 4,6-di-tert-butyl-p-cresol, CAS 497-39-2, 18.2.2000.

Other references:

Rochester CH (1971) **In:** The Chemistry of the Hydroxyl Group, part 1. Wiley, NY, p. 374 (as cited in Smith MB and March J (2001). March's Advanced Organic Chemistry, 5th edition. John Wiley and Sons, Inc., p. 330).