TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

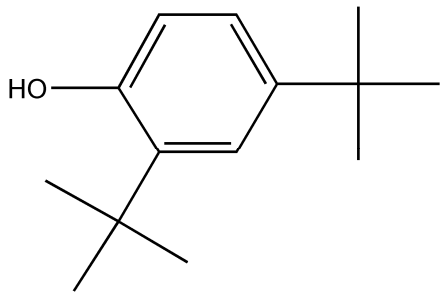
Substance name: 2,4-di-tert-butylphenol

EC number: 202-532-0

CAS number: 96-76-4

Molecular formula: C14H22O

Structural formula:



Summary of the evaluation:

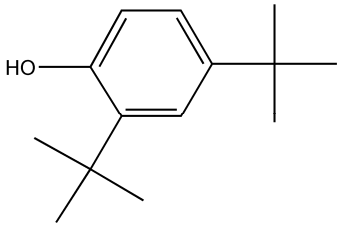
2,4-di-tert-butylphenol is not considered to be a PBT substance. This conclusion applies for the parent compound only.

The substance does not meet the B criterion. It may meet the P/vP criteria based on screening data. Although its isomer 2,6-di-tert-butylphenol (CAS 128-39-2) and a structurally similar compound 2,6-di-tert-butyl-m-cresol (BHT; CAS 128-37-0) have been observed to degrade, no estimate of the rate of degradation is available. The assessment of ecotoxicity was not completed.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: 2,4-di-tert-butylphenol
EC Number: 202-532-0
CAS Number: 96-76-4
IUPAC Name:
Molecular Formula: C14H22O
Structural Formula:



Molecular Weight: 206
Synonyms: 2,4-bis(1,1-dimethylethyl)phenol; 2,4-di-tert-butylhydroxybenzene

1.1 PURITY/IMPURITIES/ADDITIVES

No data available.

1.2 PHYSICO-CHEMICAL PROPERTIES

Table 1 Summary of physico-chemical properties

REACH ref Annex, §	Property	Value	Comments
VII, 7.1	Physical state at 20 C and 101.3 Kpa	solid liquid	Both forms are provided in European Commission (2000)
VII, 7.2	Melting / freezing point	55ºC 55.6ºC	Huels AG (1995); data not evaluated Huels AG (1994) ; data not evaluated
VII, 7.3	Boiling point	264ºC (at 1013 hPa) 265ºC (at 1013 hPa)	Huels AG (1995); data not evaluated Huels AG (1994) ; data not evaluated
VII, 7.5	Vapour pressure	0.01 hPa (at 20ºC) < 1 hPa (at 50ºC)	extrapolated from the data of Huels AG (1994); data not evaluated Huels AG (1995); data not evaluated
VII, 7.7	Water solubility	12 mg l^{-1} (at 20ºC) 11.54 (at 25ºC)	Huels AG (1994); data not evaluated WSKOW v 1.41
VII, 7.8	Partition coefficient n-octanol/water (log value)	5.13 5.33 5.19	CLOGP, Huels AG (1995); data not evaluated KOWWN v1.67 KOWWIN v1.67 exper.database; data not evaluated
	Dissociation constant	8-11	For hydroxylated aryl compounds (Rochester, 1971) (data not evaluated)

2 MANUFACTURE AND USES

Seven companies have notified the substance under Regulation 93/793/EEC. According to European Commission (2000), a quantity of 10,000-50,000 tonnes/annum is produced and/or imported in Europe. According to industry, the substance is sold solely for use as an intermediate to chemical industry for production of phenolic antioxidants and UV-stabilisers.

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

No experimental data are available on 2,4-di-tert-butylphenol. A structurally similar compound 2,6-di-tert-butyl-m-cresol (BHT; CAS 128-37-0) has been observed to oxidise in water to several transformation products with a moderate to rapid rate in the dark and under sunlight (faster degradation in sunlight) (see PBT summary fact sheet No. 121). In addition, results of Freitag et al., (1982) indicate that the isomer 2,6-di-tert-butylphenol might not be photolytically stable in some test conditions (see PBT summary fact sheet No. 13).

Indirect photochemical degradation in the atmosphere is considered to be fast based on the estimated half-life of 7.8 hours for the reaction with OH-radicals using AOP v1.91 (24-hour day^{-1}; $5*10^5$ OH^- cm^{-3}).

4.1.2 Biotic degradation

In a test according to ISO draft "BOD test for insoluble substances" from 1990, 2% biodegradation after 28 days was observed using domestic aerobic activated sludge (Huels AG, 1990). Test concentration of 34.5 mg l^{-1} was used, which is above water solubility of 2,4,-di-tert-butylphenol. The study report was not available to the Rapporteur for evaluation. CERI (2007) reports on a ready biodegradation test according to OECD 301C using a test concentration of 100 mg l^{-1} and a sludge concentration of 30 mg l^{-1}. No degradation was observed during 28 days (measured as BOD). The study report was not available to the Rapporteur for evaluation.

BIOWIN v4.02 indicates that the substance is not readily biodegradable and may be persistent in the environment (ultimate degradation predicted to take weeks to months).

The structurally similar substance BHT has been observed to be degraded in soil via biological and abiotic 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

2,4-di-tert-butylphenol is not readily biodegradable but it can be expected to be oxidised in aquatic solution and possibly be subject to biodegradation based on the data on structurally similar substance BHT. In the lack of information on the rate of primary degradation, identity of degradation products and mineralisation, no conclusion can be made on the persistence of the substance but further testing would be necessary on abiotic and biological degradation.

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

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 logKow of 5.19, a BCF 702 was derived by BCFWIN v2.15.

4.3.2 Measured bioaccumulation data[3]

MITI (1992) conducted a flow-through bioaccumulation test (according to OECD 305C) using *Cyprinus carpio*. BCF of 135-360 for 2 µg l^{-1} and BCF of 128-436 for 20 µg l^{-1} test concentrations were reported (BCFs refer to the relation of measured concentrations in water and fish over the sampling occasions during the 8 weeks of exposure period). No substance specific test details are available. The test concentrations are below the water solubility of 2,4-di-tert-butylphenol and results are independent of the test concentrations. As a conclusion, the result can be considered reliable enough for the assessment.

4.3.3 Other supporting information[4]

No data available.

4.3.4 Summary and discussion of bioaccumulation

Based on the predicted BCF and the experimental BCF in the range of 128-436, it is concluded that 2,4-di-tert-butylphenol has a moderate bioaccumulation potential.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

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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

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

The substance may volatilise, adsorb to test system surfaces or degrade in test conditions typical for testing effects. Therefore only flow-through tests and semi-static tests with test concentration monitoring are capable to produce reliable information on the effects of the test substance whereas results of static tests must be considered as less reliable.

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

In a static test according to DIN 38412 Part 15 with *Leucidus idus* a LC_{50} (48-hour) of 1.8 mg l^{-1} was observed (Huels AG, 1987). No monitoring of test concentrations occurred and due to a static system the actual test concentrations and the result may be lower than reported. The result is considered not reliable. The study report was not available to the Rapporteur for evaluation.

ECOSAR v0.99h predicts a LC_{50} (96-hour) at 0.3 mg l^{-1} for fish (logKow of 5.19 used).

Long-term toxicity

No experimental data are available. Long-chain alkyl phenols like nonyl phenol and p-tert octyl phenol are known to have endocrine disrupting properties. Also alkyl phenols with shorter alkyl chains have shown endocrine disrupting properties. For p-tert pentyl phenol there are evidence from both *in vitro* and *in vivo* studies and p-tert butyl phenol has shown affinity to the ER-receptor in vitro. The estrogen receptor affinities of 50 chemicals including 2,4-di-tert-butylphenol was investigated by Laws *et al.* (2006) using the rat uterine cytosolic ER-competitive binding assay. No IC_{50} could be determined for 2,4-di-tert-butylphenol due to solubility constraints and the inhibition of estradiol binding at the highest possible test concentration (100µM) was 20-40%. For comparison it can be noted that the EC_{50} of 17-β-estradiol was 0.00052 µM. 2,4-di-tert-butylphenol was negative in the uterotrophic bioassay (OECD, 2007).

6.1.1.2 Aquatic invertebrates

Acute toxicity

No experimental data are available. ECOSAR v0.99h predicts an EC_{50} (48-hour) at 0.6 mg l^{-1} for Daphnia (logKow of 5.19 used). This value is in the line with the experimental data on the isomer 2,6-di-tert-butylphenol (see PBT summary fact sheet No. 13).

Long-term toxicity

No experimental data are available.

6.1.1.3 Algae and aquatic plants

No experimental data are available. ECOSAR v0.99h predicts an EC_{50} (96-hour) at 0.2 mg l^{-1} (logKow of 5.19 used).

6.1.2 Sediment organisms

No data available.

6.1.3 Other aquatic organisms

Huels AG (1991) reported an EC_{50} > 1,700 mg l^{-1} obtained for *Pseudomonas putida* in a test conducted according to Huels AG own test method ("Oxygen consumption test", 1991). The study report was not available to the Rapporteur for evaluation.

6.2 TERRESTRIAL COMPARTMENT

No data available.

6.3 ATMOSPHERIC COMPARTMENT

No data available.

7 PBT AND VPVB

7.1 PBT, VPVB ASSESSMENT

Persistence: 2,4-di-tert-butylphenol may meet the P/vP criteria. The substance is not readily biodegradable but it can be expected to be oxidised in aquatic solution and be possibly subject to biodegradation based on the data on structurally similar substance BHT. Further testing would be needed to examine the rate of abiotic and biological degradation and the identity of expected transformation products. However, further testing is not required due to the overall conclusion (see below).

Bioaccumulation: 2,4-di-tert-butylphenol does not meet the B criterion. The predicted bioconcentration factor is 702 and the experimental BCF is 128-436. This conclusion applies for the parent compound, only.

Toxicity: No reliable experimental data are available for 2,4-di-tert-butylphenol. For the isomer 2,6-di-tert-butylphenol, short-term flow-through tests with fish and invertebrates are available. Two tests with invertebrates resulted EC_{50} –values close to the trigger of 0.1 mg l^{-1}. QSAR-predictions or 2,4-di-tert-butylphenol are also close to the T-criterion. No experimental data on algae are available. 2,4-di-tert-butylphenol was found to be a very weak binder to the rat estrogen receptor in an *in vitro*

assay and gave a negative result in the uterotrophic bioassay in rodents. Thus, this substance it is not considered to fulfil the T-criterion with regards to endocrine disrupting effects. For a complete assessment, chronic experimental data would be needed, but such data are not required due to the overall conclusion (see below).

Summary: The substance does not meet the B criterion. It may meet the P/vP criteria. Although its isomer 2,6-di-tert-butylphenol (CAS 128-39-2) and a structurally similar compound 2,6-di-tert-butyl-m-cresol (BHT; CAS 128-37-0) have been observed to degrade, no estimate of the rate of degradation is available. The assessment of ecotoxicity was not completed.

It is concluded that 2,4-di-tert-butylphenol is not considered as a PBT substance. This conclusion applies for 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, 2,4-di-tert-butylphenol, CAS 96-76-4, 19.2.2000.

Other references:

CERI (2007) Biodegradation and bioaccumulation data of existing chemicals. Chemicals Evaluation and Research Institute Website http://www.cerij.or.jp/ceri_en/index_e4.shtml.

Laws S, Yavanhxay S, Cooper R and Eldridge C (2006) Nature of the binding interaction of 50 structurally diverse chemicals with rat estrogen receptors. Toxicological Sciences vol. 94. No.1, 46-56.

MITI (1992) Biodegradation and Bioaccumulation data of Existing Chemicals based on CSCL Japan, Compiled under the Supervision of Chemical Products Safety Division, Basic Industries Bureau MITI, ed. by CITI, 1992. Published by Japan Chemical Industry Ecology-Toxicology & Information Center.

OECD (2007) Series on testing and assessment No. 67. Report of the validation of the uterotrophic bioassay: additional data supporting the test guideline on the uterotrophic bioassay in rodents.

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 & Sons, Inc., p. 330).