TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

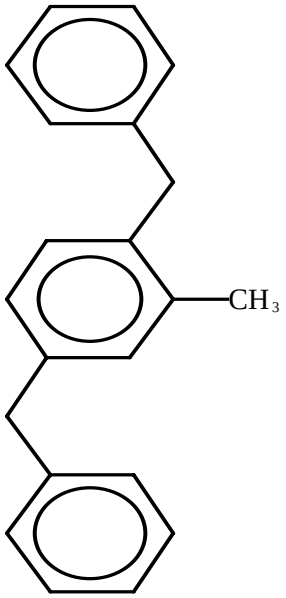
Substance name: dibenzyltoluene

EC number: 248-097-0

CAS number: 26898-17-9

Molecular formula: C21H20

Structural formula:



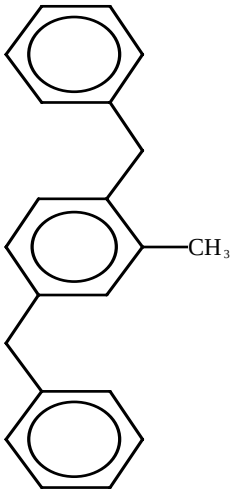
Summary of the evaluation:

Dibenzyltoluene is not considered to be a PBT substance. It does not meet the P/vP criterion based on screening data. Its predicted metabolites do not fulfil the screening P/vP criteria. Dibenzyltoluene meets the B criterion based on screening data, but its first metabolite does not fulfil the screening B criterion. Ecotoxicity assessment was not completed.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Dibenzyltoluene
EC Number: 248-097-0
CAS Number: 26898-17-9
IUPAC Name:
Molecular Formula: C21H20
Structural Formula:



Molecular Weight: 272.39
Synonyms: Benzene, methylbis(phenylmethyl)-

1.1 PURITY/IMPURITIES/ADDITIVES

True dibenzyltoluene is composed of 6 isomers whose proportions depend on reaction conditions.

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	
VII, 7.2	Melting/freezing point		
VII, 7.3	Boiling point		
VII, 7.5	Vapour pressure		
VII, 7.7	Water solubility	0.0018 mg/L < 0.1 mg l^{-1} 0.04 mg l^{-1} (at 25ºC)	ELF ATOCHEM (1995) MITI (1992); data not evaluated WSKOW v1.41
VII, 7.8	Partition coefficient n-octanol/water (log value)	6.59	KOWWIN v1.67
	Dissociation constant		

2 MANUFACTURE AND USES

One site has provided information on the substance under Regulation 93/793/EEC. According to industry, two producers operate at the moment. Based on the information gathered under Regulation 92/793/EEC, the volume produced is < 1,000 tpa. The substance is known to be used as intermediate but other uses cannot be ruled out.

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 dibenzyltoluene.

Indirect photochemical degradation in the atmosphere is considered to be fast based on the estimated half-life of 14.2 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

A test on ready biodegradability according to OECD 301 (MITI I) showed with test concentration of 100 mg l^{-1} and (predominantly domestic) sludge inoculum of 30 mg l^{-1} no degradation (0% measured as BOD/ThOD) after 28 days (MITI 1992).

A test measuring primary degradation and using conditions similar to (2-phases) closed bottle test for ready biodegradability was carried out by ATOCHEM (1990). Disappearance of dibenzyltoluene was monitored by GC and disappearance of aromatic cycles by UV-spectroscopy. In GC analysis, 65% disappearance was observed in 62 days (94% in 149 days), and UV-spectrometer measured 13 % disappearance in 20 days, 58% in 62 days, 50% in 105 days and 67% in 149 days. GC analysis refers to % degradation with respect to initial concentration, 1.5 mg/l. UV spectroscopy analysis is related to aromatic rings absorption and so measures rings disappearance.

CATABOL predicts biodegradation of 0.8% for MITI I test (OECD 301C) conditions. Probability to be metabolised is 22% (on molar basis) whereas the not metabolised quantity is predicted to be 78%. According to the CATABOL prediction, in the MITI I test conditions 22% of the parent substance (on molar basis) is metabolised to a stable metabolite presented in Figure 1. Degradation probability of this substance is 3%. Metabolites formed in the degradation pathway predicted by CATABOL are presented in Figure 2. Formation probability of degradation products with less than 3 aromatic rings is < 1%. The sixth metabolite biodegrades with a high probability comprised between 0.9 and 1. According to BIOWIN v4.00, all metabolites formed after the fifth metabolite are non persistent. For all these metabolites, results for the Primary Biodegradation Timeframe (Biowin 4) are from days/weeks to hours/days and results from the Non-Linear Model Prediction (Biowin 2) are Biodegrades fast.

Following biodegradation was predicted by BIOWIN v4.02:

Table 2 BIOWIN v4.02 predictions for dibenzyltoluene and its predicted stabile metabolite

	Dibenzyltoluene	Benzoic acid metabolite of dibenzyltoluene
Biowin 1	Biodegrades fast (1.04)	Biodegrades fast (1.15)
Biowin 2	Biodegrades fast (0.99)	Biodegrades fast (1.0)
Biowin 3	Weeks-months (2.42)	Weeks-months (2.51)
Biowin 4	Days-weeks (3.26)	Days-weeks (3.29)
Biowin 5	Biodegrades slowly (0.06)	Biodegrades slowly (0.19)
Biowin 6	Biodegrades slowly (0.02)	Biodegrades slowly (0.08)
Ready biodegradability prediction:	Not readily biodegradable	Not readily biodegradable

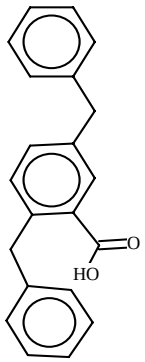


Figure 1 Benzoic acid metabolite of dibenzyltoluene.

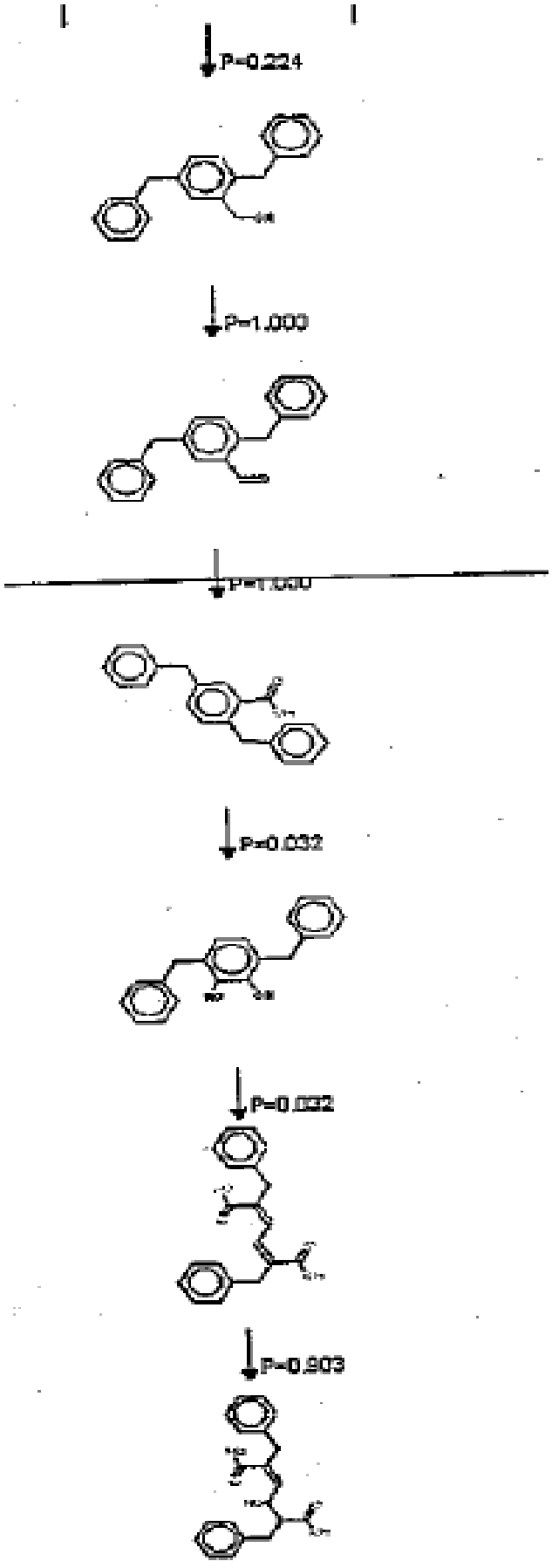


Figure 2 Metabolites formed in the degradation pathway of dibenzyltoluene based on CATABOL.

4.1.3 Other information [1]

No data available.

4.1.4 Summary and discussion of persistence

Regarding ready biodegradability, the available predictions with BIOWIN and CATABOL and the OECD 301 C test of MITI (1992) determine all the substance as not readily biodegradable. Based on BIOWIN2 and BIOWIN 3 predictions, dibenzyltoluene is not persistent. The closed bottle test of ATOCHEM (1990) observed disappearance of aromatic rings (58% by 62 days). This observation provides evidence that the substance is degraded in a reasonable time range to substances containing less than 3 aromatic rings. The test result is in conflict with the CATABOL prediction (< 1% probability for metabolites with less than 3 aromatic rings to be formed). The first metabolite predicted by CATABOL is a benzoic acid derivative. BIOWIN2 and BIOWIN3 estimates would indicate that this substance is not persistent. The metabolites predicted by CATABOL to be formed, if the benzoic acid derivative is further degraded, produce similar BIOWIN2 and BIOWIN3 estimates. Considering the combination of CATABOL (metabolite identification) and BIOWIN predictions together with the closed bottle test results, it is concluded that dibenzyltoluene is not persistent.

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 6.59, a BCF of 23,480 was derived by BCFWIN v2.15.

For the first metabolite (benzoic acid derivative) a logKow of 5.58 is estimated by KOWWIN v1.67. This value refers to the unionised form of the substance. Benzoic acids are in the environmentally relevant pH range mainly in ionised form and the corresponding logKow is likely to be considerably lower than the value predicted for unionised form. In line with this assumption, BCFWIN v 2.15 predicts a BCF of 5.6.

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

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

4.3.2 Measured bioaccumulation data[3]

MITI (1992) has reported results from a test according to OECD 305 for this CAS-number. The results were provided for four peaks (indicating that the test substance was an isomer mixture). BCF range of 1,180-8,180 with test concentration of 0.0001 mg l^{-1} and BCF range of 785-6,160 with test concentration of 0.001 mg l^{-1} were observed for "peak B". For other peaks BCF range of 590-6,190 (test conc. 0.0001 mg l^{-1}) and 301-4,020 (test conc. 0.001 mg l^{-1}) were determined during the 10-week test. It was not possible to determine the identity of single peaks. More detailed data are not available, and it is hence not possible to see whether a steady state was reached in the test. However, the reported BCF ranges indicate that the steady state BCF would be above 5,000.

Due to the unclarity regarding the identity of the peaks of the bioconcentration test, the identity of the test substance cannot be reliably connected with the substance subject to the PBT assessment. Hence, the results are not considered further.

4.3.3 Other supporting information[4]

No data available.

4.3.4 Summary and discussion of bioaccumulation

Experimental BCFs up to 8,180 were derived in a test according to OECD 305. In addition a BCF of 23,480 has been predicted for the substance. It is concluded that the substance has a very high bioaccumulation potential. The first metabolite formed is expected to have a low bioaccumulation potential based on BIOWIN-prediction (BCF = 5.6). Benzoic acids are generally not expected to bioaccumulate.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

Data on ecotoxicity was not reviewed for this report.

6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

Long-term toxicity

[3] For example, fish bioconcentration factor

[4] For example, measured concentrations in biota

6.1.1.2 Aquatic invertebrates

Acute toxicity

Long-term toxicity

6.1.1.3 Algae and aquatic plants

6.1.2 Sediment organisms

6.1.3 Other aquatic organisms

6.2 TERRESTRIAL COMPARTMENT

6.3 ATMOSPHERIC COMPARTMENT

7 PBT AND VPVB

7.1 PBT, VPVB ASSESSMENT

Persistence: Dibenzyltoluene does not meet the P/vP criteria based on screening data. The BIOWIN2 and BIOWIN 3 predictions indicate that the substance is not persistent. CATABOL predicts that the substance is not readily biodegradable but identifies a metabolite (22% of substance metabolised under MITI I test conditions), which is a benzoic acid derivative of the parent substance. This metabolite and the predicted further metabolites (with very low formation probability) do not according to BIOWIN predictions fulfil the screening P/vP criteria.

According to a standard test (OECD 301 C), dibenzyltoluene is confirmed to be not readily biodegradable (0% degradation in 28 days). The result is in line with the ready biodegradability predictions of BIOWIN and CATABOL. CATABOL predicts a very low formation probability (< 1%) for metabolites with less than 3 aromatic cycles but the prediction is in contradiction with available closed bottle test, where disappearance of aromatic cycles was observed to reach 13% in 20 days, 58% in 62 days and 67% in 149 days. Based on CATABOL information on the identity of the metabolites, BIOWIN predictions and the results of the closed bottle test, it is concluded that dibenzyltoluene is not persistent.

Bioaccumulation: Dibenzyltoluene fulfils the B criterion based on screening data (estimated logKow 6.59). The predicted first stable metabolite is benzoic acid derivative of the substance. For this substance a BCF of 5.6 is predicted for pH range relevant for the environment. Hence the first stable metabolite does not fulfil the B screening criterion.

Toxicity: Data on ecotoxicity was not reviewed for this report.

Summary: Dibenzyltoluene does not meet the P/vP criteria based on screening data. Its anticipated metabolites do not fulfil the screening P/vP criteria. Dibenzyltoluene meets the B criterion based on

screening data, but its first stable metabolite does not fulfil the screening B criterion. Assessment of ecotoxicity was not conducted. It is concluded that the substance is not considered as a PBT substance.

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 sources:

ATOCHEM (1990). Biodégradabilité aérobie primaire du JARYSOL BT 02 (dibenzyltoluène). Boutonnet JC, ATOCHEM, DRDI, Centre d'Application de Levallois, Service Analyse-Environnement, rapport n°30504 du 12/11/1990.

ELF ATOCHEM (1995) Dibenzyltoluène, détermination de l'hydrosolubilité. Thiébaud H & Brochier P. ELF ATOCHEM, DCRD, Centre d'Application de Levallois, Service Analyse-Environnement, rapport réf. 95/SAE6/0649/HT du 20/09/1995.

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.