

TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

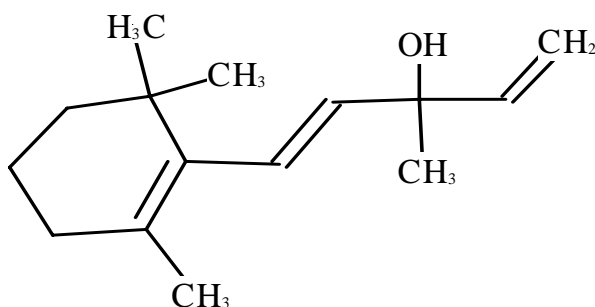
Substance name: 3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-ol

EC number: 226-006-5

CAS number: 5208-93-5

Molecular formula: C₁₅H₂₄O

Structural formula:



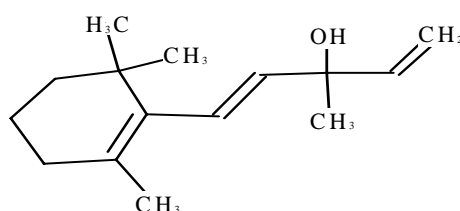
Summary of the evaluation:

The substance is not considered to be a PBT substance. It does not meet the P/vP criteria based on screening data. It may meet the B/vB criteria according to screening data. T criterion is likely to be not fulfilled but the assessment of ecotoxicity was not completed.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: 3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-ol
 EC Number: 226-006-5
 CAS Number: 5208-93-5
 IUPAC Name:
 Molecular Formula: C₁₅H₂₄O
 Structural Formula:



Molecular Weight: 220.36
 Synonyms: Vinylionol; for the complete list of synonyms, see European Commission (2000)

1.1 Purity/Impurities/Additives

No data available.

1.2 Physico-Chemical properties

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

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 Kpa	liquid	
V, 5.2	Melting / freezing point	-25°C	BASF AG (1995) (data not evaluated)
V, 5.3	Boiling point	270 °C (at 1,000 hPa)	BASF AG (1995) (data not evaluated)
V, 5.5	Vapour pressure	0.00238 hPa (at 19.7°C)	BASF AG (1989) (data not evaluated)
V, 5.7	Water solubility	151 mg l ⁻¹ (at 25°C) 2.44 mg l ⁻¹ (at 25°C)	BASF AG (1995) (data not evaluated) WSKOW v1.41
V, 5.8	Partition coefficient n-octanol/water (log value)	5.45 4.9	KOWWIN v1.67 BASF AG (1995) (data not evaluated)
VII, 5.19	Dissociation constant	-	

2 MANUFACTURE AND USES

One company has notified the substance under Regulation 93/793/EEC. According to the producer, the substance is used solely for the synthesis of vitamin A in closed systems.

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 abiotic degradation. The substance is not expected to be subject of relevant abiotic degradation in aqueous media.

Indirect photochemical degradation in the atmosphere is considered to be fast based on the estimated half-life of 1.3 hours for the reaction with OH-radicals using AOP v1.91 (24 h day⁻¹; 5*10⁵ OH⁻ cm⁻³).

4.1.2 Biotic degradation

A test on ready biodegradability according to OECD 301C (modified MITI) resulted by day 27 a degradation of 52% (BOD of ThOD). Domestic sludge and a test concentration of 92 mg l⁻¹ were used (BASF AG, 1988). It is noted that the study report was not available to the Rapporteur for evaluation.

A new ready biodegradability test according to OECD 301B (CO₂-evolution) was conducted by BASF AG (2003) in compliance with GLP. The test concentration was approximately 24 mg vinylionol l⁻¹. Activated sludge from a laboratory wastewater plant treating municipal sewage was used as inoculum (suspended solids concentration 30 mg l⁻¹). A mineralisation degree of 63% and 64% (two replicates) was achieved in 28 days but the 10-d window was not reached. Hence the substance fails to meet the criteria for ready biodegradability. The study is briefly described but seems to be of acceptable quality.

4.1.3 Other information ¹

No data available.

4.1.4 Summary and discussion of persistence

No data are available on abiotic degradation in aqueous media. Two standard ready biodegradability tests are available (BASF AG, 1988 and BASF AG, 2003). In the OECD 301C –test the pass level of ready biodegradability was almost achieved, whereas in the OECD 301B –test the overall pass level was exceeded but the 10-window not met. It can be concluded that the substance is not readily biodegradable but can be considered as not persistent.

4.2 Environmental distribution

Data not reviewed for this report.

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

4.2.1 Adsorption

4.2.2 Volatilisation

4.2.3 Long-range environmental transport

4.3 Bioaccumulation (B)

4.3.1 Screening data²

A measured logK_{ow} of 4.9 and an estimated logK_{ow} of 5.45 are available for the substance. BCFWIN v2.14 provides a BCF of 1,183 using the first value and a BCF of 3,162 using the latter value.

4.3.2 Measured bioaccumulation data³

No experimental data on bioaccumulation are available for the substance.

4.3.3 Other supporting information⁴

No data available.

4.3.4 Summary and discussion of bioaccumulation

No experimental data on bioaccumulation are available. Based on the experimental logK_{ow} of 4.9, it is concluded that the substance has a high bioaccumulation potential. Testing would be necessary to determine the actual bioaccumulation potential

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

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)

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

A LC₅₀ (96 hours) of 2.2 mg l⁻¹ was obtained according to DIN 38 412 method (static) for *Leuciscus idus* (BASF AG, 1989). It is noted that the test report was not available for the Rapporteur for evaluation.

Long-term toxicity

No data available.

6.1.1.2 Aquatic invertebrates

Acute toxicity

For *Daphnia magna* an EC₅₀ (48 hours) at 0.81 mg l⁻¹ was determined by BASF AG (1989) according to DIN 38 412/11. Test substance had a purity of 92.9% and a solvent was used. It is noted that the test report was not available for the Rapporteur for evaluation.

Long-term toxicity

No data available.

6.1.1.3 Algae and aquatic plants

An EC₅₀(96h) of 6.5 mg l⁻¹ referring to biomass and an EC₅₀ (96 hours) of 11.1 mg l⁻¹ referring to growth rate were obtained for *Scenedesmus subspicatus* in a test according to DIN 38 412/9 by BASF AG (1989). Test substance had a purity of 92.9% and a solvent was used. It is noted that the test report was not available for the Rapporteur for evaluation.

6.1.2 Sediment organisms

No data available.

6.1.3 Other aquatic organisms

Data available for effects on micro-organisms were not reviewed for this report.

6.2 Terrestrial compartment

No data available.

6.3 Atmospheric compartment

No data available.

7 PBT AND vPvB

7.1 PBT, vPvB assessment

Persistence: 3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-ol does not meet the P/vP criteria based on screening data. The substance failed to meet the 10-d window in a standard ready biodegradability test (OECD 301B) but reached in 28 days > 60% biodegradation level. In addition, it just failed the pass level of ready biodegradability in an OECD 301C -test. Hence, the substance is considered as biodegradable although it is not readily biodegradable.

Bioaccumulation: the substance may meet the B/vB criteria according to screening data. The available experimental logKow is 4.9, which is above the screening trigger of 4.5. Further testing would be necessary to determine the actual bioaccumulation potential. However, such testing is not needed in the frame of this assessment due to the overall conclusion (see below).

Toxicity: no long-term data are available on the effects of the substance to biota. The very few short term aquatic data indicate that the substance may not meet the T criterion. Long-term testing would be necessary to complete the assessment of ecotoxicity. However, such testing is not needed in the frame of this assessment due to the overall conclusion (see below).

Summary: 3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-ol does not meet the P/vP criteria based on screening data. It may meet the B/vB criteria according to screening data. The assessment of ecotoxicity was not completed. 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 source:

European Commission (2000) IUCLID Dataset, 4-(2,4-dichlorophenoxy)aniline, CAS 14861-17-7, 18.2.2000.

BASF (2003) Vinyljonol G, determination of the biodegradability in the CO₂-evolution test. Project No.:03/0145/36/2