

TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

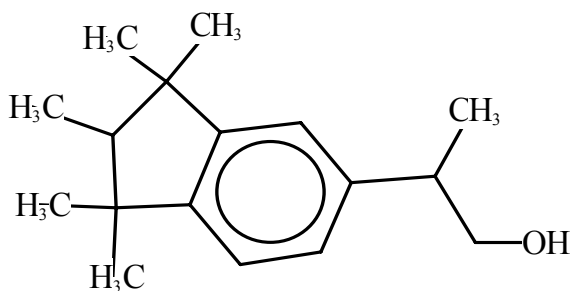
Substance name: β ,1,1,2,3,3-hexamethylindan-5-ethanol

EC number: 214-934-3

CAS number: 1217-08-9

Molecular formula: C₁₇H₂₆O

Structural formula:



Summary of the evaluation:

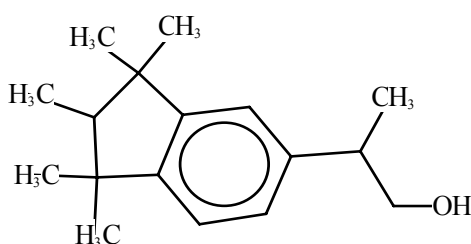
β ,1,1,2,3,3-hexamethylindan-5-ethanol is not considered to be a PBT substance. It does not meet the B criterion based on data of a structurally similar substance, 1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethylindeno(5,6-c)pyran (CAS 1222-05-5; PBT Summary No. 02). Assessment of persistency and ecotoxicity was not conducted for this report.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: β ,1,1,2,3,3-hexamethylindan-5-ethanol
 EC Number: 214-934-3
 CAS Number: 1217-08-9
 IUPAC Name:
 Molecular Formula: C₁₇H₂₆O

Structural Formula:



Molecular Weight: 246.40
 Synonyms: Galaxolide alcohol; 1H-Indene-5-ethanol, 2,3-dihydro-.beta.,1,1,2,3,3-hexamethyl-

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
V, 5.1	Physical state at 20 C and 101.3 Kpa	liquid	
V, 5.2	Melting / freezing point	-	
V, 5.3	Boiling point	-	
V, 5.5	Vapour pressure	-	
V, 5.7	Water solubility	1.278 mg l ⁻¹ (at 25°C)	WSKOW v1.41
V, 5.8	Partition coefficient n-octanol/water (log value)	5.62	KOWWIN v1.67
VII, 5.19	Dissociation constant	-	

2 MANUFACTURE AND USES

Two companies have provided information on the substance under Regulation 93/793/EEC. The substance is used solely as an intermediate in synthesis of 1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethylindeno(5,6-c)pyran (CAS 1222-05-5; HHCB). The use volume is according to industry < 1,000 tonnes/annum at the present.

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.

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; $5 \cdot 10^5 \text{ OH}^- \text{ cm}^{-3}$).

4.1.2 Biotic degradation

No data available.

4.1.3 Other information ¹

No data available.

4.1.4 Summary and discussion of persistence

No experimental data on abiotic or biotic degradation are available for the substance. The assessment of persistency was not carried out for this report.

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

An estimated logK_{ow} of 5.62 is available for the substance (KOWWIN v1.67.) Using this value, BCFWIN v2.14 provides a BCF of 944.8, whereas the recalculated Connel model (recommended by TGD) provides a BCF of 23,010. It is noted that BCFWIN does not recognize the aliphatic cyclic structure of the chemical, but only corrects the basic equation for the fragment aromatic ring with alkylalcohol.

For the structurally related substance 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno(5,6-c)pyran (see Figure 1; PBT Summary No. 02; HHCB), an experimental logK_{ow} of 5.3 has been chosen as a representative value (European Commission, 2006). However, the estimated logK_{ow} for this substance is 6.62 (KOWWIN v1.67).

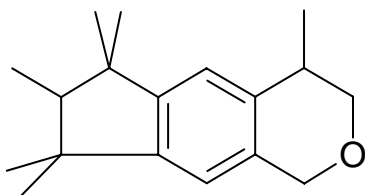


Figure 1. Structural formula of 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno(5,6-c)pyran (CAS 1222-05-5)

4.3.2 Measured bioaccumulation data³

No experimental data on bioaccumulation are available for the substance.

Based on reliable experimental BCFs for *Brachydanio rerio* and *Lepomis macrochirus* and BAFs derived from concentrations measured in field, BCFs between 600 and 1,600 (parent compound) have been considered representative for fish for HHCB. In addition, metabolites of HHCB have been followed in a study with *Lepomis macrochirus*. The fish were observed to biotransform the substance and excrete the metabolites fast. A BCF below 2,000 for the parent and metabolites together was determined. Additionally, measured environmental data on HHCB from several predatory species including mammals confirm, that the substance is not accumulating in the food chain (European Commission, 2007; see also PBT Summary No. 02).

As HHCB is biodegrading, the main primary biodegradation products identified have been scrutinised regarding their bioaccumulation potential with a result that they have logK_{ow} ≤ 4. Further degradation products are due to their increasing polarity expected to have lower logK_{ow} than the identified primary degradation products (European Commission, 2007).

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

³ For example, fish bioconcentration factor

4.3.3 Other supporting information⁴

No data available.

4.3.4 Summary and discussion of bioaccumulation

No experimental data on bioaccumulation are available for β ,1,1,2,3,3-hexamethylindan-5-ethanol. The substance is structurally similar with 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno (5,6-c)pyran (HHCB; CAS 1222-05-5; PBT Summary No. 02). For this substance a solid experimental dataset is available with representative BCFs of 600-1,600 for fish for the parent compound. Furthermore, BCF of HHCB is below 2,000 for the parent compound and fish metabolites in total. The biodegradation products of HHCB have a $\log K_{ow} \leq 4$.

The estimated $\log K_{ow}$ of β ,1,1,2,3,3-hexamethylindan-5-ethanol is lower than the estimated $\log K_{ow}$ of HHCB. Therefore, and due to the structural similarity, the bioaccumulation potential of β ,1,1,2,3,3-hexamethylindan-5-ethanol is not expected to be higher than the bioaccumulation potential of HHCB.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

No experimental data are available for the substance.

6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

Long-term toxicity

6.1.1.2 Aquatic invertebrates

Acute toxicity

Long-term toxicity

⁴For example, measured concentrations in biota

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: No experimental data on degradation are available for β ,1,1,2,3,3-hexamethylindan-5-ethanol. The assessment of persistence was not conducted for this report.

Bioaccumulation: β ,1,1,2,3,3-hexamethylindan-5-ethanol does not fulfil the B criterion based on experimental bioaccumulation data of the structurally similar substance 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno(5,6-c)pyran (CAS 1222-05-5; HHCB) This substance, its metabolites (in fish) and degradation products do not fulfil the B criterion (see European Commission, 2007 and PBT Summary No. 02).

Toxicity: No experimental data are available on the effects of the substance to biota. The assessment of ecotoxicity was not carried out for this report.

Summary: β ,1,1,2,3,3-hexamethylindan-5-ethanol does not meet the B criterion based on the data on the structurally similar substance 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno(5,6-c)pyran (CAS 1222-05-5). No assessment of persistency and ecotoxicity was carried out for this report. 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:

European Commission (2000) IUCLID Dataset, β ,1,1,2,3,3-hexamethylindan-5-ethanol, CAS 1217-08-9, 18.2.2000.

European Commission (2007) European Risk Assessment Report, Draft of July 2007, HHCB, CAS No: 1222-05-5, EINECS No: 214-946-9.