TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

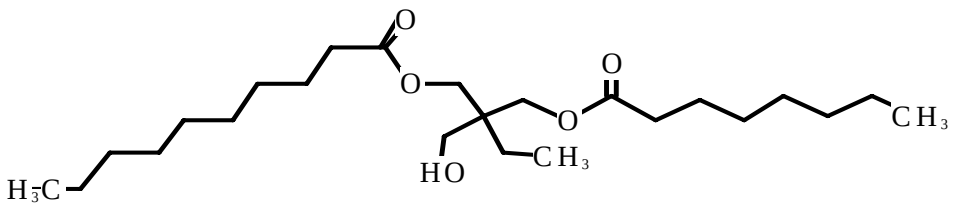
Substance name: Decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol octanoate

EC number: 234-392-1

CAS number: 11138-60-6

Molecular formula: C24H46O5

Structural formula:



Summary of the evaluation:

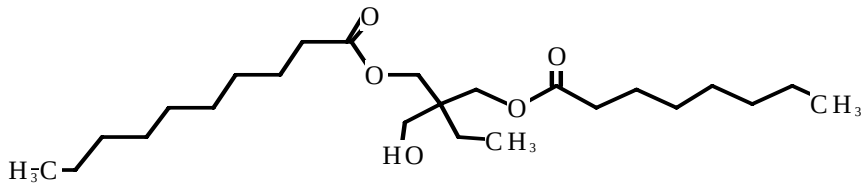
Decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol octanoate is not considered to be a PBT substance. It does not meet the P/vP criteria based on screening data. It may meet the B/vB criteria according to screening data. The assessment of ecotoxicity was not completed.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name:	Decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol octanoate
EC Number:	234-392-1
CAS Number:	11138-60-6
IUPAC Name:	
Molecular Formula:	C24H46O5

Structural Formula:



Molecular Weight:	414.63
Synonyms:	TMP tricaprylate/caprate; trimethylolpropane esters of C8/C10 fatty acids; 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	-45ºC (pour point)	Unichema Chemie B.V. (data not evaluated)
V, 5.3	Boiling point	> 200ºC (at 1000 hPa)	Unichema International (data not evaluated)
V, 5.5	Vapour pressure	< 1 hPa (at 20ºC)	Unichema International (data not evaluated)
V, 5.7	Water solubility	0.0023 mg l^{-1} (at 25ºC)	WSKOW v1.41
V, 5.8	Partition coefficient n-octanol/water (log value)	7.67 > 3	KOWWIN v1.67 Unichema International (data not evaluated)
VII, 5.19	Dissociation constant	-	

2 MANUFACTURE AND USES

Five companies have notified the substance under Regulation 93/793/EEC. The production and import volume is according to European Commission (2000) 5,000-10,000 tpa.

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 14.5 hours for the reaction with OH-radicals using AOP v1.91 (24 h day^{-1}; $5*10^5$ OH^- cm^{-3}).

4.1.2 Biotic degradation

In an OECD 301B test with non-adapted sludge and a test substance concentration of 9.8 mg l^{-1} 21.6% was degraded (measured as CO_2 evolution) in 28 days when the sample was not shaken (Unichema Chemie B.V.). A similar study with agitated samples gave a degradation of 45.6% based on CO_2 evolution (Unichema Chemie B.V.). A third study performed according to EEC directive 79/831 annex V part C 5.2 with 100 mg l^{-1} test substance resulted in 18.5% degradation after 35 days (Unichema Chemie B.V). All three studies indicate that the substance is not readily biodegradable. An additional study performed according to CEC L-33-T-82 with 50 mg l^{-1} test substance gave 98-100% degradation after 7 days (Unichemca Chemie B.V.). It is noted that reports of these tests were not available to the Rapporteur for evaluation.

A ready biodegradability study according to OECD 301B (CO_2-evolution) resulted a mineralisation of > 60% in 28 days (Unilever, 1994). The 10-days window was reached. The test is considered valid with restrictions mainly because the test report did not specify the medium used and whether the test was performed in the darkness. Furthermore, the temperature variation was too wide.

In addition, two ready biodegradability studies are reviewed (references not known) by ACC (2001). One study performed according to EPA 560/6-82-003 (equivalent to OECD 301B, CO_2-evolution test) using two different concentrations resulted in 64 and 67% degradation, respectively, during 27 days at 25°C. The 10-days window criterion was not met. This study is ranked as being not reliable by ACC (2001), because it was not performed in the darkness and yeast was added to the inoculum. Another study according to OECD 301 ranked as being valid without restrictions gave 76% degradation during 28 days but the 10-day window criterion was not met. The rapporteur has not reviewed these two studies.

4.1.3 Other information [1]

No data available.

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

4.1.4 Summary and discussion of persistence

No experimental data are available on abiotic degradation of the substance. The substance reached in one standard ready biodegradability test (Unilever, 1994) according to OECD 301B the trigger for ready biodegradability. However, this test is not completely reliable. The other results available from standard tests indicate that biodegradation occurs but that the substance is not readily biodegradable. It is concluded that the substance it is expected to biodegrade in the environment although it is considered to be not readily biodegradable.

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]

An estimated logKow of 7.67 (KOWWIN v1.67) is available for the substance. Using this value, BCFWIN v2.14 provides a BCF of 247.7, whereas the recalculated Connel model (recommended by TGD) provides a BCF of 33,884.

4.3.2 Measured bioaccumulation data[3]

No experimental data on bioaccumulation are available for the substance.

4.3.3 Other supporting information[4]

No data available.

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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

4.3.4 Summary and discussion of bioaccumulation

No experimental data on bioaccumulation are available. Based on the estimated logKow of 7.67 and the contradicting BCF-estimates, it can be expected that the substance has a moderate to high bioaccumulation potential. Testing would be necessary to determine the actual bioaccumulation potential.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

No long-term experimental ecotoxicity data are available for the substance. The available aquatic acute tests as cited by ACC (2001) for daphnia, fish and algae are limit tests conducted far above the water solubility. However, it is noted, that no effects were observed in these tests, which would indicate low acute ecotoxicity. The test reports were not available to the Rapporteur for evaluation.

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

6.1.1.3 Algae and aquatic plants

6.1.2 Sediment organisms

No data available.

6.1.3 Other aquatic organisms

Data 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: decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol octanoate does not meet the P/vP criteria based on screening data. The substance was not readily biodegradable in most of the standard biodegradability screening tests available, but a sufficient degree of degradation was reached to conclude that the substance is not persistent due to its biodegradability.

Bioaccumulation: the substance may fulfil the B/vB criteria according to screening data. The available estimated logKow is 7.67, which is above the screening trigger of 4.5. Testing would be necessary to determine the actual bioaccumulation potential. However, such testing is not required in the frame of this assessment due to the overall conclusion (see below).

Toxicity: no long-term experimental data are available on the effects of the substance to biota. Very few short-term limit tests are available, but they were not evaluated by the Rapporteur and hence no conclusion has been derived. Long-term testing would be necessary to complete the assessment of ecotoxicity. However, such testing is not required in the frame of this assessment due to the overall conclusion (see below).

Summary: decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol octanoate 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 sources:

European Commission (2000) IUCLID Dataset, Decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol octanoate, CAS 11138-60-6, 18.2.2000.

ACC (2001) HPV Chemical challenge program. Test plan for aliphatic esters category, provided by American Chemistry Council.