TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVP SUBSTANCES

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

Substance name: 2-Propenoic acid, 2-methyl-, C9-11-isoalkyl esters, C10-rich

EC number: 292-128-0

CAS number: 90552-07-1

Molecular formula: C₁₄H₂₆O₂

Structural formula:

Summary of the evaluation:

At the current state of knowledge, the substance is not considered to be a PBT substance. It does not meet the P or vP criteria. It does meet the screening criteria for B and there is insufficient information to assess whether the T criterion is met.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name:	2-Propenoic acid, 2-methyl-, C9-11-isoalkyl esters, C10-rich
EC Number:	292-128-0
CAS Number:	90552-07-1
IUPAC Name:	
Molecular Formula:	$C_{14}H_{26}O_2$
Molecular Weight:	226
Structural Formula:	

Synonyms:	Isodecyl Methacrylate	
	Methacrylic Acid, Isodecyl Ester	
	2-Methyl-2-propenoic acid, isoalkyl esters	
	C9-C11-isoalkyl methacrylates	
	C9-C11-isoalkyl-2-methyl-2-propenoate	
	C9-C11-isoalkyl-2-methylpropenoates	
	Methacrylic acid, C9-C11 isoalkyl esters	

1.1 Purity/Impurities/Additives

1.2 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	120°C at 3.99hPa, >250°C at 1013hPa	Result from IUCLID, not reviewed
V, 5.5	Vapour pressure		
V, 5.7	Water solubility	0.01 mg/l	Result from IUCLID, not reviewed
V, 5.8	Partition coefficient n- octanol/water (log value)	4.92	HPLC method
			Result from IUCLID, not reviewed
VII, 5.19	Dissociation constant		

Table 1Summary of physico-chemical properties

2 MANUFACTURE AND USES

Not relevant.

3 CLASSIFICATION AND LABELLING

This substance is not currently listed on Annex I of the Dangerous Substances Directive 67/548/EEC.

3.1 Degradation (P)

3.1.1 Abiotic degradation

No data available.

3.2 Biotic degradation

IUCLID contains a summary of a modified MITI test which showed 50.4 % biodegradation after 28 days. In a new study supplied by industry (not included in IUCLID but which has been reviewed), 88% degradation was observed in a 28 day OECD 301B Sturm test. The 10 day window was not met, but the level of degradation observed suggests that the substance is not persistent. In addition,

BIOWIN predicts that the substance would degrade quickly, with ultimate degradation within weeks.

3.2.1 Other information ¹

3.2.2 Summary and discussion of persistence

The results of biodegradation tests, together with BIOWIN predictions, indicate that, whilst not readily biodegradable, the substance is biodegraded to a significant extent in 28 days and is unlikely to be persistent.

3.3 Environmental distribution

- 3.3.1 Adsorption
- 3.3.2 Volatilisation

3.4 Bioaccumulation (B)

3.4.1 Screening data²

The Log Kow measured by HPLC method is 4.92 (data from IUCLID).

3.4.2 Measured bioaccumulation data³

No data available.

3.4.3 Other supporting information⁴

3.4.4 Summary and discussion of bioaccumulation

The Log Kow of 4.92 indicates that the screening criterion for B is met. Bioaccumulation potential has not been assessed further since the substance is not considered to be persistent.

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

 $^{^2}$ For example, log $K_{\rm ow}$ values, predicted BCFs

³ For example, fish bioconcentration factor

⁴For example, measured concentrations in biota

3.5 Secondary poisoning

4 HUMAN HEALTH HAZARD ASSESSMENT

According to data in the IUCLID file, which have not been peer reviewed, this substance has low acute oral toxicity with LD50s in rats of >5000 mg/kg bw. There are no valid data for repeated dose toxicity or developmental toxicity/teratogenicity listed in IUCLID.

5 ENVIRONMENTAL HAZARD ASSESSMENT

5.1 Aquatic compartment (including sediment)

5.1.1 Toxicity test results

5.1.1.1 Fish

Acute toxicity

IUCLID lists a 48h LC50 for Leuciscus idus of 470 mg/l. This data has not been peer reviewed and the result is greatly in excess of the reported water solubility. Toxicity has not been assessed further since the substance is not considered to be persistent.

Long-term toxicity

No data available in IUCLID.

5.1.1.2 Aquatic invertebrates

Acute toxicity

No data available in IUCLID.

Long-term toxicity

No data available in IUCLID.

5.1.1.3 Algae and aquatic plants

No data available in IUCLID.

5.1.2	Sediment organisms
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- 5.1.3 Other aquatic organisms
- 5.2 Terrestrial compartment
- 5.3 Atmospheric compartment
- 5.4 Indirect exposure via the food chain

6 PBT AND VPVB

6.1 **PBT**, vPvB assessment

Persistence: the level of degradation observed in a 28 day OECD 301B Sturm test, 88%, indicates that the P and vP criteria are not met.

Bioaccumulation: The Log Kow of 4.92 indicates that the screening criterion for B is met. Bioaccumulation potential has not been assessed further since the substance is not considered to be persistent.

Toxicity: The only ecotoxicity data available is a fish 48h LC50 of 470 mg/l. The study has not been peer reviewed. Toxicity has not been assessed further since the substance is not considered to be persistent.

Summary: this substance does not meet the P or vP criteria and so is not considered a PBT substance according to the EU criteria. It does meet the screening criteria for B and there is insufficient information to assess whether the T criterion is met.

INFORMATION ON USE AND EXPOSURE

Not relevant as substance is not identified as a PBT.

OTHER INFORMATION

The information used in this report was taken from the following sources: Publicly available IUCLID file, 2000.