TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

Substance name: Ethanol, 2,2'-iminobis-, N-C12-18-alkyl derivs.

EC number: 276-014-8

CAS number: 71786-60-2

Molecular formula: not applicable

Structural formula: not applicable

Summary of the evaluation:

Ethanol, 2,2'-iminobis-, N-C12-18-alkyl derivs is not considered as 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:	Ethanol, 2,2'-iminobis-, N-C12-18-alkyl derivs.
EC Number:	276-014-8
CAS Number:	71786-60-2
IUPAC Name:	
Molecular Formula:	not applicable
Structural Formula:	not applicable
Molecular Weight:	not applicable
Synonyms:	N,N-Bis(2-hydroxyethyl)-C12-18-alkylamine

1.1 PURITY/IMPURITIES/ADDITIVES

The substance consists of primary alkylamines with two ethylalcohol groups. The chain length of the alkyl fragments is between C12 and C18 according to the information from industry.

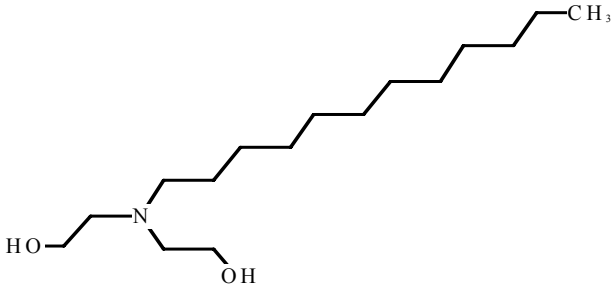

Figure 1. A constituent with C12-alkyl chain fragment.

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		Only calculated values are available:
		83.13 mg l^{-1} (at 25ºC) (C12-derivative)	WSKOW v1.41
		0.822 mg l^{-1} (at 25ºC) (C16-derivative)	WSKOW v1.41
		0.081 mg l^{-1} (at 25ºC) (C18-derivative)	WSKOW v1.41
V, 5.8	Partition coefficient n-octanol/water (log value)		Only calculated values are available:
		3.9 (C12-derivative)	KOWWIN v1.67
		3.94 (C12-derivative)	SPARC
		4.23 (C12-derivative)	ClogP
		5.86 (C16-derivative)	KOWWIN v1.67
		5.79 (C16-derivative)	SPARC
		6.09 (C16-derivative)	ClogP
		6.85 (C18-derivative)	KOWWIN v1.67
		6.7(C18-derivative)	SPARC
		7.02 (C18-derivative)	ClogP
VII, 5.19	Dissociation constant	approximately 8.8 (calculated)	APAG (2003)

The constituents are weak bases with surfactant properties. Based on the estimated pKa of 8.8, a large part of the substance is present in protonated form in environmentally relevant pH range (approximately 4-9).

2 MANUFACTURE AND USES

One company has provided information on the substance under Regulation 93/793/EEC.

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 for the substance on abiotic degradation.

Indirect photochemical degradation in the atmosphere is considered to be very fast based on the estimated half-life of approximately 13 minutes for all constituents for the reaction with OH-radicals using AOP v1.91 (24 h day^{-1}; $5 \cdot 10^5$ OH^- cm^{-3}).

4.1.2 Biotic degradation

A test on ready biodegradability according to OECD 301C (modified MITI I) resulted a degradation of 8% in 28 days (cited as "Synprolam 35 x 2." in European Commission, 2000). The study report was not available to the Rapporteur for evaluation. It is noted, that the test substance contains several constituents and hence the result does not necessarily reflect biodegradation rate of all constituents.

A study of ultimate biodegradability by the ISO standard 14593 resulted in a mineralisation expressed as 37% of the theoretical IC yield (ICI). A safety data sheet for the substance (Clariant, 2003), states that the degradation is 47% in a study according to OECD guideline 301E. A closed bottle test with the constituent octadecylbis(2-hydroxyethyl)amine gave > 60% degradation in 28 days (van Ginkel and Kroon, 1993). Further to this, safety data sheets for the related substances bis(2-hydroxyethyl)cocoalkylamine, CAS No. 61791-31-9 (Akzo Nobel, 2002) and N-alkyl tallow N,N-bishydroxyethylamine, CAS No. 61791-44-4 (CECA, 2002) state biodegradation > 60% as BOD in 28 days (in OECD 301 D) and 76% biodegradability after 28 days (in OECD 301 F) for the two substances, respectively. None of these studies has been reviewed by the Rapporteur.

BIOWIN v4.02 predicts for the constituent with **C12-fragment** following biodegradation: BIOWIN2 = 0.73, BIOWIN3 = 2.96, BIOWIN6 = 0.91. For the constituent with **C16-fragment** the results are: BIOWIN2 = 0.55, BIOWIN3 = 2.83, BIOWIN6 = 0.91. For the constituent with **C18-fragment** the results are: BIOWIN2 = 0.80, BIOWIN3 = 2.77, BIOWIN6 = 0.92. All three constituents are predicted to be biodegradable and the rate of biodegradation is not clearly dependent on the alkyl chain length.

4.1.3 Other information [1]

No data available.

4.1.4 Summary and discussion of persistence

No experimental data are available on abiotic degradation of the substance. According to the ready biodegradability tests with the whole multi-constituent substance, it can be concluded that the substance does not pass the criteria of ready biodegradability. However, the level of degradation observed in the tests shows that the substance is biodegradable. Standard ready biodegradability tests with two related multi-constituent mixtures support this conclusion. It must be nevertheless

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

noted that results from tests using multi-constituent substances as test material do not necessarily reflect the degradation of each constituent.

The constituent octadecylbis(2-hydroxyethyl)amine is according to the available closed bottle test readily biodegradable. Hence, looking at the results obtained with the whole multi-constituent substance, it could be expected that other constituents are biodegraded more slowly, although BIOWIN predicts approximately equally fast rate of degradation for constituents with C12-, C16 and C18 –fragments. However, BIOWIN supports the impression, that all constituents would be biodegrading although the whole substance does not reach the criterion for ready biodegradability.

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]

The constituents of the substance are basic surfactants with pKa values around 8.8. The substances are present in the environmentally relevant pH range largely in protonated form. Due to the surface active properties, octanol water partitioning is not a good surrogate for their adsorption or bioaccumulation potential. Therefore the use of QSARs relating logKow to BCF is not appropriate.

The QSAR of Meylan et al. (1999) used by BIOWIN v4.02 predicts for ionic substances containing alkyl chains with ≥ 11 carbons a 1.85 ≤ log BCF ≤ approximately 2.2. As these values have been obtained using a model developed on a basis of experimental data, the values automatically take the approximate degree of ionisation into account in environmentally relevant pH -range. For the latter logKow -value, the corresponding BCF is 158. However, this method delivers many underestimations of BCFs compared to measured values and the sub-training set for ionic substances with long alkyl chains included only 5 compounds. Hence, this QSAR-method is not reliable for estimating the bioaccumulation potential of the substance.

4.3.2 Measured bioaccumulation data[3]

No data available.

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

3 For example, fish bioconcentration factor

4.3.3 Other supporting information[4]

No data available.

4.3.4 Summary and discussion of bioaccumulation

No experimental data are available on bioaccumulation potential of the substance. The constituents of the substance are surfactants and present in the environment largely in cationic form. Hence, its adsorption and bioaccumulation potential cannot be predicted by their octanol-water partitioning. In addition, the only available QSAR-method for ionic substances (BCFWIN) is not reliable for substances with long alkyl chains. Testing of single constituents or a realistic worst case representative of the constituents would be necessary to determine the actual bioaccumulation potential.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

The acute toxicity of the substance to rainbow trout has been estimated according to OECD guideline 203 giving a nominal 96-hour LC_{50} of 0.36 mg/l (ICI). In addition to this, a safety data sheet (Clariant, 2003) states a 96-hour LC_{50} of 0.6 mg/l for zebra fish.

It must be noted, that the results reflect ecotoxicity of the whole multi-constituent substance and that some of the constituents may exhibit considerably higher toxicity if measured separately.

A safety data sheet for the related substance bis(2-hydroxyethyl)cocoalkylamine states a 96-hour LC_{50} for zebra fish to be 0.28 mg/l (Akzo Nobel, 2002).

Long-term toxicity

No experimental data are available.

[4]For example, measured concentrations in biota

6.1.1.2 Aquatic invertebrates

Acute toxicity

One daphnia study according to OECD 202 gave a nominal 48h-EC_{50} of 0.6 mg/l (ICI). It must be noted, that the results reflect ecotoxicity of the whole multi-constituent substance and that some of the constituents may exhibit considerably higher toxicity if measured separately.

In a safety data sheet for the related substance bis(2-hydroxyethyl)cocoalkylamine a 48-hour EC_{50} for daphnia of 0.84 mg/l is reported (Akzo Nobel, 2002). For another related substance , N-alkyl tallow N,N bis hydroxy ethylamine, a safety data sheet reports a 48-hour EC_{50} of < 1mg/l for daphnia (CECA, 2002).

Long-term toxicity

No data available.

6.1.1.3 Algae and aquatic plants

No experimental data are available.

6.1.2 Sediment organisms

No data available.

6.1.3 Other aquatic organisms

No data available.

6.2 TERRESTRIAL COMPARTMENT

No data available.

6.3 ATMOSPHERIC COMPARTMENT

No data available.

7 PBT AND VPVB

7.1 PBT, VPVB ASSESSMENT

Persistence: Ethanol, 2,2'-iminobis-, N-C12-18-alkyl derivs. does not meet the P/vP criteria based on screening data. The substance is not readily biodegradable but it and its constituents are expected to be biodegradable based on screening biodegradation tests with one constituent (octadecylbis(2-hydroxyethyl)amine), with the substance itself, with related multi-constituent substances and based on QSAR-predictions of the constituents.

Bioaccumulation: The substance may meet the B/vB criteria according to screening data. No experimental data are available for the substance. Due to the surfactant and ionic nature of the

constituents, logKow is not a good predictor of bioaccumulation and adsorption potential. Further testing is necessary to determine the actual bioaccumulation potential. However, such testing is not required due to the overall conclusion (see below).

Toxicity: No experimental long-term ecotoxicity data are available for the substance or its constituents. Short-term tests with fish and invertebrates are available for the substance and related multi-constituent substances indicating that the substance might not fulfil the T criterion. In order to complete the assessment, long-term effects data for constituents representing realistic worst case ecotoxicity are necessary. However, further testing is not required due to the overall conclusion (see below).

Summary: Ethanol, 2,2'-iminobis-, N-C12-18-alkyl derivs. 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, Ethanol, 2,2'-iminobis-, N-C12-18-alkyl derivs., CAS 71786-60-2, 19.2.2000.

Other sources:

Akzo Nobel (2002) Safety data sheet for Ethomeen C/12 (CAS No. 61791-31-9).

APAG (2003) Comments provided by APAG to the PBT assessment.

CECA (2002) Safety data sheet for Noramox S 2/ Noroplast 8000 (CAS No. 61791-44-4).

Clariant (2003) Safety data sheet for Genamin S 020 Special (CAS No. 71786-60-2).

Ginkel CG van and Kroon AGM (1993) Metabolic pathway for the biodegradation of octadecyl (2-hydroethyl)amine. Biodagradation 3, 435-443.

ICI report – ISO 14593 evaluation of ultimate aerobic biodegradability as cited by Uniquema, comments and data provided to the Rapporteur in March, 2003.

ICI reports on acute fish and daphnia tests according to OECD guidelines No. 203 and No. 202 as cited by Uniquema, comments and data provided to the Rapporteur in March, 2003.