TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

Substance name: Sulphonic acids, C10-21-alkane, Ph esters

EC number: 293-728-5

CAS number: 91082-17-6

Molecular formula: not applicable

Structural formula: not applicable

Summary of the evaluation:

The main constituents of sulphonic acids, C10-21-alkane, Ph esters are not considered as PBT. They do not meet the P/vP criteria based on screening data but they meet the screening B criteria. This UVCB substance contains impurities, which may meet the P/vP and B/vB criteria based on screening data. These impurities are, however, present in such low concentrations (0.005-0.008% w/w each; sum conc. of all < 1% w/w) that they are not considered to be of concern at present due to a very limited potential for environmental release from the current production and use within the EU. This conclusion applies, unless a substantial increase in environmental release occurs in future. Assessment of ecotoxicity was not carried out during this assessment.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Sulphonic acids, C10-21-alkane, Ph esters
EC Number: 293-728-5
CAS Number: 91082-17-6
IUPAC Name:
Molecular Formula: not applicable
Structural Formula: not applicable
Molecular Weight: not applicable
Synonyms: Alkane C10-C21 sulphonic acid phenyl esters

1.1 PURITY/IMPURITIES/ADDITIVES

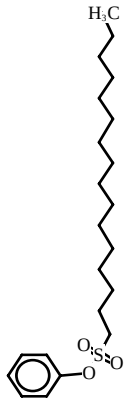
Sulphonic acids, C10-21-alkane, Ph esters belongs to the group of UVCBs. The composition as compiled from the descriptions of Bayer AG (2003a,b,c; 2004 and 2007):

Consituent/impurity	Concentration (% w/w)
Linear alkane-mono-sulfonic acid mono-phenylesters ("monoesters")	approximately 70
Linear alkane-di-sulfonic acid di-phenylesters ("diesters")	20 - 25
Linear alkane-tri-sulfonic acid tri-phenylesters ("triesters")	approximately 4
Minor linear alkane sulphonic acid phenylesters	0.5 - 2
Sulphonic acid phenylesters with branched alkanes:	< 1.0 in total
with cyclic alkane groups (e.g. cyclohexane ring) in the middle of the paraffin chain	0.3 - 0.4
with aromatic groups (e.g. a benzene ring) in the middle of the paraffin chain	< 0.01
With single branching in the paraffin chain	< 0.5
with fully branched paraffin chain	< 0.1

Based on the purity of the paraffin used as a starting material in the production of the substance, it can be expected that alkane fragments of the constituents of sulphonic acids, C10-21-alkane, Ph esters consist mainly of linear C14-C17 chains. Only minor amounts (up to approximately 2% w/w) of linear C10-C13 and C15-C20 paraffins are present in this multi-component substance. The content of linear paraffins in the starting material is normally 99.1 – 99.3% w/w. A representative species of the linear paraffin fraction of sulphonic acids, C10-21-alkane, Ph esters is hexadecane-1-sulphonic phenylester (CAS 94245-73-5; see Figure 1).

The concentrations of the impurities included in the minor branched fraction have been estimated based on the purity of the starting material. This fraction contains 30-40 substances in a concentration range of 50-80 ppm (0.005–0.008%) each.

Figure 1 Structural formula of a linear constituent
hexadecane-1-sulphonic acid phenylester



1.2 PHYSICO-CHEMICAL PROPERTIES

Table 1 Summary of physico-chemical properties. For details and 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	< -15ºC	Bayer AG data (data not evaluated)
V, 5.3	Boiling point	approximately 200ºC (at 13 hPa) (decomposes)	Bayer AG data (data not evaluated)
V, 5.5	Vapour pressure	< 0.0001 hPa (at 20ºC)	Bayer AG data (data not evaluated)
V, 5.7	Water solubility	2 mg l^{-1} (at 22ºC)	Bayer AG data (data not evaluated)
V, 5.8	Partition coefficient n-octanol/water (log value)	> 6	CLOGP (Bayer AG, 1992; data not evaluated; no details provided on for which component the estimation was carried out)
VII, 5.19	Dissociation constant	-	

Water solubility and logKow predicted for some constituents and impurities are presented in **Table 4.2**, Section 4.3.1.

2 MANUFACTURE AND USES

One producer has provided information on the substance. Its production volume in Europe is in the range of 10,000 to 20,000 tonnes/annum (GDCh, 1996 and 2006).

The substance is produced in two phases. The starting material for the synthesis is a paraffin product, which is a mixture of linear C14-C17 paraffins (for impurity information, see Section 1.1). In the first reaction steps, secondary sulfonylchlorides of the paraffin mixture are formed. These react in the second step with sodium phenolate to alkane sulfonic acid phenylesters. The product is purified by neutralisation, washing and distillation (Bayer AG, 2003a).

3 CLASSIFICATION AND LABELLING

The substance is not included 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 sulphonic acids, C10-21-alkane, Ph esters.

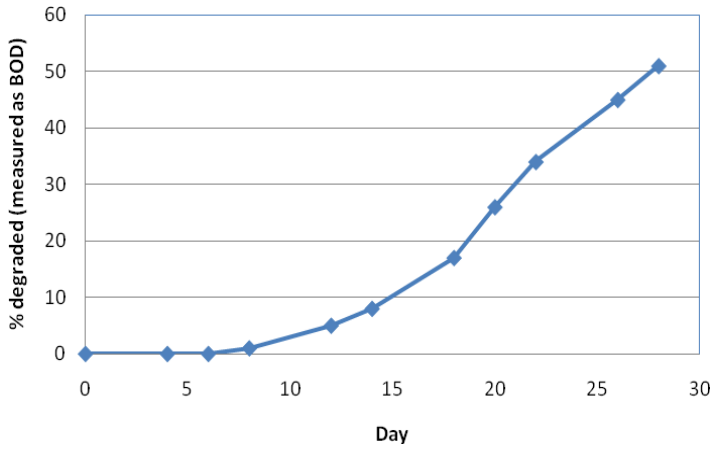
For hexadecane-1-sulphonic acid phenylester (HDSAP), one of the linear constituents, indirect photochemical degradation in the atmosphere is considered to be fast based on the estimated half-life of 9.1 hours for the reaction with OH-radicals using AOP v1.91 (24-hr day^{-1}; $5 \cdot 10^5$ $OH^- cm^{-3}$).

4.1.2 Biotic degradation

A modified MITI test on ready biodegradability according to Directive 84/449/EEC C.7 has been conducted by Bayer AG (Bayer AG data). Predominantly domestic sludge and a test concentration of 100 mg l^{-1} were used. In 28 days a degradation of 30% was observed (measured as O_2 consumption). It is noted that the study report was not available to the Rapporteur for evaluation. It is concluded that on the basis of the test the substance (as a complex mixture) is not readily biodegradable.

A model substance hexadecane-1-sulphonic acid phenylester (CAS 94245-73-5) representing the linear paraffin constituents of sulphonic acids, C10-21-alkane, Ph esters was tested according to Directive 92/69/EEC C.4-D (similar to OECD 301F) (Bayer AG, 2003d). Predominantly domestic sludge was employed. The degradation proceeded as presented in **Figure 4.1**.

Figure 4.1 Biodegradation of hexadecane-1-sulphonic acid phenylester (CAS 94245-73-5) (Bayer AG, 2003d)



A long lag phase was followed by a steady increase of the amount degraded to the point of test termination. The degradation plateau was not reached. Based on the amount degraded by day 28 (51%), it is expected that the 60% degradation level (pass level for readily biodegradable) would have been reached within the following week. The test is considered valid. No inhibition of the

microbial biomass at test concentration level (100 mg l^{-1}) seemed to have occurred and the reference substance was appropriately degraded. On the basis of the test it is concluded that the constituent is biodegradable but just fails to reach the pass level of ready biodegradability. Thus this constituent does not fulfil the (v)P criteria. Although other linear constituents with longer C-chain may be less water soluble and may need more time for degradation, they are based on their structural similarity with HDSAP also not considered to be fulfilling the (v)P criteria.

Persistence of some "monoester" constituents and impurities has been predicted by BIOWIN v 4.02 (see **Table 4.1**).

Table 4.1 Predicted persistency of some "monoester" constituents and impurities.

Constituent or impurity (named according to the paraffin fragment) Smiles	BIOWIN 2	BIOWIN 3	BIOWIN 6	Screening (v)P criteria of TGD fulfilled?
Linear C10- CCCCCCCCCCS(=O)(=O)(Oc1ccccc1)	0.84	2.86	0.17	No
Fully branched C10- CC(C)(C)C(C)(C)C(C)(C)S(=O)(=O)(Oc1ccccc1)	0.01	1.93	0.02	Yes
Linear C14- CCCCCCCCCCCCCCS(=O)(=O)(Oc1ccccc1)	0.83	2.74	0.18	No
Branched C14- (1 double branching, 3 single)	0.12	2.23	0.01	Yes (limit)
Branched C14- (2 double branches and 2 single branches)	0.02	2.01	0.01	Yes
Linear C15- CCCCCCCCCCCCCCCS(=O)(=O)(Oc1ccccc1)	0.81	2.71	0.19	No
Fully branched C15- C(C)(C)C(C)(C)C(C)(C)C(C)(C)C(C)(C)S(=O)(=O)(Oc1ccccc1)	0.00	1.6	0.00	Yes
Linear C16- CCCCCCCCCCCCCCCCS(=O)(=O)(Oc1ccccc1)	0.77	2.67	0.19	No
Linear C21- CCCCCCCCCCCCCCCCCCCCCS(=O)(=O)(Oc1ccccc1)	0.56	2.51	0.21	No
Fully branched C21- C(C)(C)C(C)(C)C(C)(C)C(C)(C)C(C)(C)C(C)(C)C(C)(C)C(C)(C)S(=O)(=O)(Oc1ccccc1)	0.00	0.95	0.00	Yes

4.1.3 Other information [1]

No data available.

4.1.4 Summary and discussion of persistence

The substance is according to a standard modified MITI–test not readily biodegradable (30% degraded in 28 days; Bayer AG data). Hexadecane-1-sulphonic acid phenylester (CAS 94245-73-5), a linear constituent of the substance, just failed to reach the pass level of a readily biodegradable

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

substance in a ready biodegradability test according to Directive 92/69/EEC C.4-D (Bayer AG, 2003d). Considering the BIOWIN –predictions of linear "monoester" constituents, hexadecane-1-sulphonic acid phenylester can be accepted to represent the biodegradation behaviour of all linear constituents of sulphonic acids, C10-21-alkane, Ph esters. Based on the test result and the BIOWIN predictions it is concluded that the linear constituents are not persistent.

Branched impurities are considered based on BIOWIN predictions to be potentially persistent.

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]

Predicted logKow, BCF and water solubility of some "monoester" constituents and impurities are presented in **Table 4.2**. Based on these estimates, it can be expected that all constituents and impurities have a logKow > 5. The logKow-value seems to depend mainly on the number of carbon atoms in the paraffin fragment. Degree of branching also has some influence to the logKow. Branching has a significant impact on the BCF-prediction of BCFWIN, which contains fragment corrections for branching.

Table 4.2 Predicted water solubility, logKow and BCF of some "monoester" constituents

Constituent/impurity	Water solubility (mg l^{-1} at 25ºC) (WSKOW v1.41)	LogKow (KOWWIN v1.67)	BCF (BCFWIN v2.15)	BCF (according to TGD)
Linear C10-	0.15	5.77	552	16,014
Fully branched C10-	0.29	5.44	3,057	8,395
Linear C14-	0.0014	7.7	202	
Branched C14- (1 double branching, 3 single)		7.4	18,190	
Branched C14- (2 double branches and 2 single branches)		7.4	20,480	
Linear C15-	0.0005	8.2	43	19,459
Fully branched C15-		7.7	6,954	32,853
Linear C16-	0.00014	8.72	9.1	
Linear C21-	$4 \cdot 10^{-7}$	11.2	3	9
Fully branched C21-	$2 \cdot 10^{-6}$	10.4	3	126

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

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.

4.3.4 Summary and discussion of bioaccumulation

No experimental data on bioaccumulation of the substance or its constituents and impurities are available. Based on the BCF–values estimated by BCFWIN, sulphonic acid monophenylesters with branched paraffin chain are expected to have a high to very high bioaccumulation potential. BCFWIN is considered more appropriate model than the models recommended by TGD for this type of substances as it takes in the prediction into account the influence of paraffin chain length and branching. Even the BCFWIN model may, however, not provide reliable BCF predictions, because the correction rules of the model are very simple. The selected constituents and impurities of this multi-constituent substance, on which predictions have been made, may be not sufficiently covered by the training set chemicals of the model (i.e. the predictions may well be outside the applicability domain of also the BCFWIN model). For monoester constituents with linear alkane chains BCFWIN predicts very low bioaccumulation potential, whereas the recalculated Connell model (recommended by TGD for substances with logKow > 6) provides a very high BCF except for the constituents with logKow of approximately 10 or higher (also the domain limit). Experimental bioaccumulation data would be necessary to determine more reliably the bioaccumulation potential. However, testing of the substance as a whole seems not analytically feasible due to the multitude and the large concentration range of the constituents and impurities in the substance. The most important candidates for testing would be the impurities with highly branched alkane fragments.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

Acute ecotoxicity data are available on sulphonic acids, C10-21-alkane, Ph esters for fish, daphnia, algae and micro-organisms (European Commission, 2000). These data were not evaluated for this report. For the main constituents and impurities no experimental data are available. Prediction of ecotoxicity for single constituents and impurities is possible only for those substances with logKow lower than 6-8 (depending on the QSAR-model chosen). Hence, it is not possible to characterise in a representative way the ecotoxicity of the constituents and impurities of the substance by modeling.

[3] For example, fish bioconcentration factor

[4] For example, measured concentrations in biota

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 evaluated 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: Sulphonic acids, C10-21-alkane, Ph esters does not meet the P/vP criteria based on screening data of its main constituents. The main constituents, which have a linear alkane fragment, are not persistent based on BIOWIN–predictions (see **Table 4.1**) and based on results of a standard (Directive 92/69/EEC method C.4-D) ready biodegradability test with hexadecane-1-sulphonic acid phenylester (a representative of the linear constituents). Hexadecane-1-sulphonic acid phenylester,

which was degraded to 51% in 28 days (without reaching the plateau), just fails to reach the pass level of ready biodegradability.

Impurities with higher and fully branched alkane fragments are considered fulfilling the screening P/vP criteria based on BIOWIN estimates. Further testing would be necessary to fully assess the degradation rate of these impurities. According to the only present European producer, these impurities are each present in a concentration of 0.005–0.008% w/w in the substance. The sum concentration of impurities with fully branched fragments is < 0.1% w/w and of impurities with any branched fragment is < 1% w/w. Due to the current production, use and the expected very low environmental emissions this fraction is not considered as concern unless a substantial increase in environmental release would occur in future. Further testing of degradation is therefore not currently required.

Bioaccumulation: The substance may meet the B/vB criteria based on screening data of its main constituents and impurities. The predicted logKow –values of the main constituents (containing a linear alkane fragment) are all > 5. Further assessment and testing would be necessary to determine more precisely or reliably the bioaccumulation potential of these constituents, but it is not required in the frame of the PBT-assessment because these constituents do not meet the screening P/vP criteria.

According to the predicted logKow -values and BCF estimates of BCFWIN, impurities with higher and fully branched alkane fragments meet the B/vB screening criteria. These impurities are also potentially persistent and therefore experimental data on their bioaccumulation potential would be necessary to complete the PBT -assessment. However, these impurities are not considered to be a concern at present due to their low concentrations in the substance and due to the very limited environmental emission of the substance (see above under “Persistence” for details).

Toxicity: No experimental ecotoxicity data are available for the constituents or impurities of the substance. QSAR-models cannot exhaustively predict ecotoxicity of the main constituents and impurities and hence it is not possible to determine whether the screening criterion would be exceeded. Testing of “worst case” constituents and impurities would be necessary to complete the assessment of ecotoxicity. Testing of the constituents with linear alkane fragments is, however, not required in the frame of this assessment, because these do not fulfil the screening P/vP criteria. In addition, testing of those branched impurities fulfilling the screening P/vP and B/vB criteria is not required at present due to the very low concentrations of each impurity in the substance and due to the very limited environmental emission of the substance (see discussion under “Persistence”).

Summary: The main constituents of sulphonic acids, C10-21-alkane, Ph esters do not meet the P/vP criteria based on screening data. These constituents fulfil the screening B/vB criteria. The substance contains impurities, which may fulfil the P/vP and B/vB criteria based on screening data, but these are present in such low concentrations (0.005-0.008% w/w each; sum conc. of all < 1% w/w), that they are not considered to be of concern unless a substantial increase in environmental release will occur in future. Ecotoxicity of the substance, its constituents or impurities was not evaluated during this assessment.

It is concluded that the main constituents of sulphonic acids, C10-21-alkane, Ph esters are not considered as PBT, but the substance contains potential PBT/vPvB impurities in a concentration < 1% w/w in total. These impurities are, however, not considered to be of concern at present due to the very limited environmental release from the current production and use. A further assessment is not warranted unless the environmental exposure increases significantly in future.

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:

Bayer AG (2003a) Email of 12.06.2003 to Henrik Tyle and Jack deBruijn (with attachment).

Bayer AG (2003b) Email of 21.7.2003 to Henrik Tyle and Jack deBruijn.

Bayer AG (2003c) Email of 21.10.2003 to Henrik Tyle and Jack deBruijn (with attachment).

Bayer AG (2003d) GPW 4763. Biodegradation. Study number 1292 A/03R, CAS 94245-73-5. 2003-12-19.

Bayer AG (2004) Email of 16.04.2004 to Henrik Tyle and Jack deBruijn (with attachment).

Bayer AG (2007) Email of 30.11.2007 to Johanna Peltola-Thies (with attachment).

European Commission (2000) IUCLID Dataset, sulphonic acids, C10-21-alkane, Ph esters, CAS 91082-17-6, 18.2.2000.

GDCh (2006) BUA Report Nr. 263, Supplementary reports XII. Edited by: Gesellschaft deutscher Chemiker, advisory committee on Existing Chemicals (BUA).

GDCh (1996) BUA Report Nr. 180, Sulfonic acids, C10-21-alkane, phenylesters. Edited by: Gesellschaft deutscher Chemiker, advisory committee on Existing Chemicals (BUA).