TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

Substance name: Alkanes, C9-12-iso-

EC number: 292-459-0

CAS number: 90622-57-4

Molecular formula: not applicable

Structural formula: not applicable

Summary of the evaluation:

Alkanes, C9-12-iso is not considered to be a PBT substance. Selected 2- to 4-branched constituents of this UVCB-substance do not meet the P/vP criteria based on screening data. The predicted biodegradation products of these constituents (corresponding alcohols and acids) are not expected to have high bioaccumulation potential. Possible 5-branched constituents are not PBT (see PBT summary no. 62). No final conclusion was drawn for the bioaccumulation potential and ecotoxicity for the parent substance.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name:	Alkanes, C9-12-iso-
EC Number:	EC number: 292-459-0
CAS Number:	90622-57-4
IUPAC Name:	
Molecular Formula:	Not applicable
Structural Formula:	Not applicable
Molecular Weight:	Not applicable
Synonyms:	Actrel 3338L
	Actrel 3356D
	Actrel 3356L
	Actrel R
	Esco Kaltreiniger X4
	Isopar G
	Isopar H
	Isoalkanes

1.1 Purity/Impurities/Additives

Alkanes, C9-12-iso- ("Isoalkanes") is considered as a UVCB substance based on the descriptions below. Two mixtures, Isopar G and H, are sold under the CAS number 90622-57-4, which slightly deviate from each other by composition (see Table 1.1).

Table 1.1 Average composition of ISOPAR G and H (Comber, 2005). *

Constituents/impurities	C8 % w/w	C9 % w/w	C10 % w/w	C11 % w/w	C12 % w/w	C13 % w/w	C14 % w/w	Others % w/w
Isopar G	0.1	0.5	53	43	4.0	0.1	0.1	2.0
Isopar H	0.2	0.2	1.0	38	60	0.6	0.2	0.1

*The values provided in Table 1.1 are rough averages and may vary up to ± 10 % w/w.

According to the hydrocarbon solvent producers (Comber, 2005), the actual composition may be different from batch to batch within a specific producer and vary from producer to producer, depending upon the actual feedstock used to prepare the product. The average Isopar H branching is 3.25 (average number of branches/molecule). Following estimates for the number of different branches have also been provided:

C	0.6
CH	2
CH2	4.2
CH3	5.3

Furthermore, the producers have provided information, that 5-15 % w/w of the substance consists of cyclic alkanes, typically C6 with varying degrees of branching.

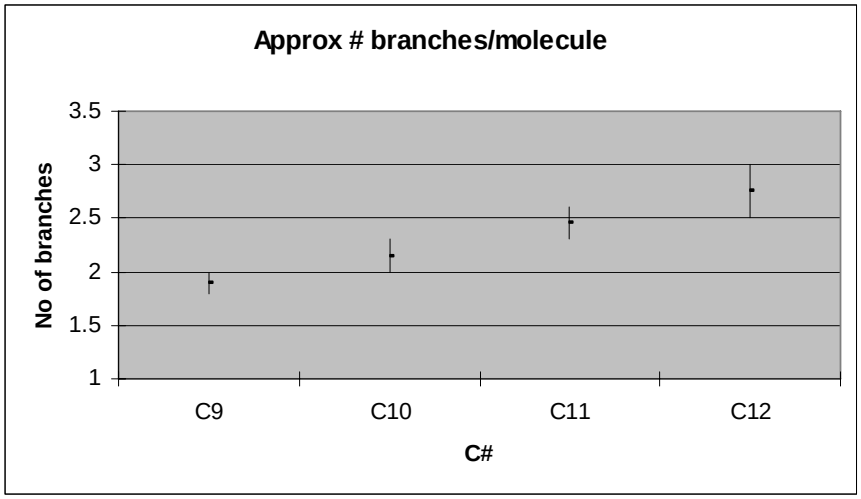

Figure 1. Number of branches in C9-C12 –constituents on the basis of more recent information (Comber, 2006).

Typical representatives as identified by the producers are presented in section 4 in connection with QSAR-predictions.

1.2 Physico-Chemical properties

Table 1.2 Summary of physico-chemical properties. For details and references, see European Commission (2000).

REACH ref Annex, §	Property	Value	Comments
VII, 7.1	Physical state at 20 C and 101.3 Kpa	Liquid	European Commission, 2000
VII, 7.2	Melting / freezing point	- 50 °C	Exxon Chemical Belgium (data not evaluated)
VII, 7.3	Boiling point	153-193 at 1013.25 hPa	Exxon Chemical Belgium (data not evaluated)
VII, 7.5	Vapour pressure	0.66 hPa at 20 °C 1.8 hPa at 20 °C	Exxon Chemical Belgium (grade Isopar H)(data not evaluated) Exxon Chemical Belgium (grade Isopar G)(data not evaluated)
VII, 7.7	Water solubility	3.11 mg l^{-1} at 25 °C < 0.1 mg l^{-1} at 20 °C ca. 85 µg l^{-1} (Isopar G) ca. 40 µg l^{-1} (Isopar H) See section 4.3.1	Estimate (WSKOW v1.41) Exxon Chemical Belgium (data not evaluted) Solubility in the test medium of 21 – day Daphnia –test, gas saturation method (EMBSI, 2004) Solubility in the test medium of 21 – day Daphnia –test, gas saturation method (EMBSI, 2004)
VII, 7.8	Partition coefficient n-octanol/water (log value)	4.61 4.9-6.9 See section 4.3.1	Estimate (KOWWIN v1.67) ASTER computer program (1995)
	Dissociation constant	-	

2 MANUFACTURE AND USES

Two producers/importers have provided data under Regulation 93/793/EEC. C3 and C4 –olefins are used as feedstock for the production of isoalkanes (Comber, 2003). The production/import volume is in the range of 100 000 t/a and the substance is used in a large variety of industrial and consumer applications according to the information provided under Regulation 93/793/EEC.

3 CLASSIFICATION AND LABELLING

The substance is not classified under Directive 67/548/EEC.

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation (P)

4.1.1 Abiotic degradation

4.1.2 Biotic degradation

Isopar G was used as test substance in an OECD 301 F –test of EMBSI (1997). With non-acclimated inoculum, 31 % was observed to be degraded after 28 day and 41 % at day 41. Using acclimated inoculum 42 % was degraded at day 28 and 48 % at day 41.

Another OECD 301 F -study with **Isopar G** showed 21.9 % degradation after 28 days using predominantly domestic sewage (EMBSI, 1995).

EMBSI (1998) carried out a ready biodegradation test (OECD 301F) with **Isopar H** as test substance. Using a non-acclimated inoculum, 6 % was degraded after 28 d, whereas with acclimated inocula 16 % was degraded by day 28 and 48 % by day 90.

The three test rows described above indicate, that Isopar H and G are not readily biodegradable, although they seem to be to some extent biodegradable also when non-adapted inocula are used. It is noted, that the test reports where not available to the Rapporteur for evaluation.

Comber (2006) provided an overview of newer biodegradation studies with Isopar G and Isopar H. Test concentration of 50 mg l^{-1} was used, whereas as degradation medium local pond water and seawater collected from Hawaii were employed, respectively for both products. The degradation conditions corresponded aerobic ready biodegradation –tests, whereas sealed flasks were used to avoid loss via volatilisation. The flasks were amended with 1 % Bushnell-Haas medium to provide ~100mM biologically available nitrogen and phosphorus. Biodegradation was monitored over time by purge-and-trap GC-MS analysis meaning that the parent compound concentration (=disappearance) was followed. For Isopar G tested in fresh water medium, loss of 99.96 % took place in 45 days, whereas in seawater 99.19 % had disappeared in 49 days. For Isopar H disappeareance of 98.13 % occurred in 45 days in freshwater and 97.7 % in 49 days in sea water. It is noted, that details of the study were not available to the Rapporteur for evaluation and it cannot

be judged based on available information how well the observed disappearance represents primary degradation. For this type of volatile and highly adsorbing substances especially recovery rates of controls are necessary background information in the evaluation of the plausibility of the results.

Due to the complexity of the substance, it is necessary to scrutinize also the biodegradation potential of constituents, as the results obtained for the multi-constituent products may not be representative for especially those constituents present in lower concentrations in the mixture. In Table 4.1 biodegradation potential has been predicted for selected constituents which are expected by the producers to be typical representatives in the substance. Additionally, some realistic worst case constituents have been considered.

Table 4.1 Biodegradation estimates of typical constituents and realistic worst case constituents (marked with asterisk) as proposed by FIN and DK (Comber, 2006).

	Smiles of the "typical" constituent	BIOWIN2* Probability**	BIOWIN3 Predicted rating***	BIOHCWIN**** DT_{50} (d)	CATABOL****** DT_{50} (d)
C9	CC(C)C(C)CCCC	0.954	3.214		
	CC(C)(C)CCCCC	0.611	3.002		
C10	CCC(C)CCCC(C)C	0.680	2.9		
	CCCCCCC(C)(C)C	0.752	3.0		
C11	CC(C)(C)CCCCCCC	0.713	3.2	10.4	9.1
	C(C)CCC(C)CCC(C)C	0.933	2.9	15	34
	CCCCC(C)C(C)C(C)C	0.933	3.2	12	20
	CCCCC(C)CC(C)(C)C	0.713	2.9	17	23
	CC(C)(C)CCCC(C)(C)C*	0.066	2.4	29	17
	CC(C)(C)CC(C)CC(C)C*	0.282	2.6	20	21
C12	CCCCC(C)CC(C)CCC	0.919	3.12	12	8
	CCCCC(C)CC(C)C(C)C	0.919	3.12	14	14
	CCCCC(C)CCC(C)(C)C	0.671	2.91	20	36
	CC(C)CCCCCCC(C)C*	0.643	2.82	12	16
	CC(C)(C)CCCCC(C)(C)C*	0.054	2.4	33	10
Napthenics (cyclic)	C1CCC(CCC)CC1	0.771	2.92	10	13.4
	C1C(C)CC(C)C(C)C1	0.771	2.92	3.5	43
	C1CC2CCCCC2CC1	0.740	2.89	69	65
	C1C(CCC)CC(CC)CC1	0.694	2.86	8	16
	C1CC(C(C)C)CCC1(C(C)C)*	0.650	2.83	12	334

* Calculated by the Rapporteur

** A biodegradation probability greater than 0.5 is considered as "biodegrades fast". A biodegradation probability less than 0.5 is considered as " does not biodegrades fast".

***Predicted Rating	Time Required for Biodegradation
5.0	hours
4.5	hours - days

4.0	days
3.5	days - weeks
3.0	weeks
2.5	weeks - months
2.0	months
1.0	longer

**** Howard (2005)

***** Results of the OECD 301F –model of CATABOL

It is noted, that the BIOCHWIN –model significantly under-predicts the degradation half-lives of isoalkanes especially those having branches at the end(s) of the alkyl chain.

CATABOL predicts that all included constituents are degraded via the same degradation route to corresponding alcohols and subsequently to acids (Comber, 2006). The training set of CATABOL is considered to cover well enough the isoalkanes in question.

The presence of penta-branched alkanes in the substance cannot be excluded. However, the relevant representatives of these have been assessed in the PBT summary no. 62.

4.1.3 Other information [1]

4.1.4 Summary and discussion of persistence

According to the available results from standard ready biodegradability studies with non-adapted and adapted inocula, Isopar G and Isopar H are considered as not readily biodegradable. However, some degradation was observed in all tests available. No degradation simulation data are available. BIOWIN2 and BIOWIN3 -predictions for typical and realistic worst case constituents with 2 to 4 branches indicate, that they are not persistent. Assessment of penta-branched alkanes has been presented in PBT summary no. 62. All constituents are predicted by CATABOL to be degraded first to corresponding alcohols and then to acids.

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

4.2 Environmental distribution

4.2.1 Adsorption

4.2.2 Volatilisation

4.2.3 Long-range environmental transport

4.3 Bioaccumulation (B)

4.3.1 Screening data

Experimental data on logKow are not available for the substance. Predicted values of logKow, water solubility and BCFs of typical and realistic worst case constituents are presented in Table 4.2.

Table 4.2 Screening bioaccumulation data of typical constituents and worst case constituents as chosen by FIN and DK (Comber, 2006).

	Smiles of the "typical" constituent	Water solubility (WSKOW v1.41) (mg l^{-1} at 25 ºC)	logKow (KOWWIN v1.67)**	BCFWIN v2.16	BCF maximal***
C9	CC(C)C(C)CCCC	3.11	4.61	712	
	CC(C)(C)CCCCC	2.90	4.65	760	
C10	CCC(C)CCCC(C)C	1.04	5.11	539	
	CCCCCCC(C)(C)C	0.97	5.14	574	
C11	CC(C)(C)CCCCCCC	0.32	5.63	1286	1560
	C(C)CCC(C)CCC(C)C	0.34	5.60	1371	1470
	CCCCC(C)C(C)C(C)C	0.40	5.52	1129	2160 (out of domain)
	CCCCC(C)CC(C)(C)C	0.37	5.56	1203	940
	CC(C)(C)CCCC(C)(C)C*	0.40	5.52	1126	1205
	CC(C)(C)CC(C)CC(C)C*	0.43	5.49	1056	191
C12	CCCCC(C)CC(C)CCC	0.11	6.09	3072	1270
	CCCCC(C)CC(C)C(C)C	0.13	6.01	2697	2650
	CCCCC(C)CCC(C)(C)C	0.12	6.05	2874	1680
	CC(C)CCCCCCC(C)C*	0.11	6.09	3072	2190
	CC(C)(C)CCCCC(C)(C)C*	0.13	6.01	2689	5980
Napthenics (cyclic)	C1CCC(CCC)CC1	3.42	4.58	665	384
	C1C(C)CC(C)C(C)C1	4.56	4.43	513	404
	C1CC2CCCCC2CC1	6.45	4.20	340	453

	C1C(CCC)CC(CC)CC1	0.44	5.48	1054	2980
	C1CC(C(C)C)CCC1(C(C)C)*	0.19	5.83	1940	4080

** Calculated by the Rapporteur

*** Model description in Dimitrov et al. (2005). This model considers factors which cause a lower bioaccumulation potential than predicted by conventional models. E.g., data on metabolism is taken into account in this model.

It must be noted, that for hydrocarbons with a logKow > 4.8, the BCFWIN v2.16 has been updated from BCFWIN v2.14 with a correction of -0.5 of the logBCF (Stewart et al., 2005). The updated hydrocarbon database of BCFWIN v2.16 contains 83 hydrocarbons including PAHs, napthenics, benzenes, alkanes, alkenes, terphenyls and olefins.

The biodegradation products (corresponding alcohols and acids) predicted by CATABOL are not expected to have relevant bioaccumulation potential.

4.3.2 Measured bioaccumulation data

Two experimentally derived BCFs have been derived from dietary studies with fish. No further information is available on the test details. It is noted, that BCFs obtained from dietary studies may overestimate the actual bioaccumulation potential.

Table 4.3 Experimentally derived BCF –values of two isoalkanes.

Compound	Log Kow	Predicted BCF	Fish species	BCF (l/kg wet)	Reference
2,3 dimethylheptane (C9)	4.6	713	Rainbow Trout	1842	Parkerton et al 2001
Dimethyldecane (C12)	6.0	9715	Rainbow Trout	2500	Parkerton et al 2001

The experimental data available for pentamethylheptanes are presented in PBT summary no. 62.

4.3.3 Other supporting information[2]

4.3.4 Summary and discussion of bioaccumulation

Two experimental BCF-values (1842 and 2500) for expected constituents of the substance are available from dietary studies with fish. These indicate high bioaccumulation potential, but it is noted, that BCF-values derived from this type of tests may overestimate the bioaccumulation potential. Predicted logKow –values of all “typical” and realistic worst case constituents indicate high bioaccumulation potential. However, the BCFWIN-model updated for hydrocarbons and another BCF-model, which takes into account the potential of, e.g., fish to metabolise the substance predict, that only certain compounds, i.e., C12-isoalkanes would possess a high or very high

[2]For example, measured concentrations in biota

bioaccumulation potential. The predicted biodegradation products (corresponding alcohols and acids) are not expected to have high bioaccumulation potential

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 Aquatic compartment (including sediment)

IUCLID of the substance contains acute ecotoxicity data for crustaceans and fish. The results are unbounded values far above the water solubility of the substance and far above the expected acute toxicity based on QSAR-predictions. Therefore, these data are not presented in the following sections.

No experimental data are available on the ecotoxicity of single constituents of the substance. Due to the variability of the branching and number of carbons of the constituents it is, however, necessary to evaluate ecotoxicity of constituents. In the following, QSAR-predictions on the ecotoxicity of several possible constituents are presented. All calculations have been carried out using the Narcosis Target Lipid Model of McGrath et al. (2004)

Table 6.1 QSAR-predictions of the ecotoxicity of typical constituents and worst case constituents as chosen by FIN and DK (Comber, 2006).

	Smiles of the "typical" constituent	Fish, NOEC (µg l^{-1})	Daphnids, NOEC (µg l^{-1})	Algae NOEC (µg l^{-1})
C9	CC(C)C(C)CCCC	46	48	
	CC(C)(C)CCCCC	24	25	
C10	CCC(C)CCCC(C)C	22	23	
	CCCCCCC(C)(C)C	15	15	
C11	C(C)CCC(C)CCC(C)C	14	15	6
	CC(C)(C)CCCCCCC	11	12	5
	CCCCC(C)C(C)C(C)C	17	18	8
	CCCCC(C)CC(C)(C)C	12	13	6
	CC(C)(C)CCCC(C)(C)C*	13	14	6
	CC(C)(C)CC(C)CC(C)C*	15	16	7
C12	CCCCC(C)CC(C)CCC	12	12	5
	CCCCC(C)CC(C)C(C)C	12	13	6
	CCCCC(C)CCC(C)(C)C	11	11	5
	CC(C)CCCCCCC(C)C*	12	12	6
	CC(C)(C)CCCCC(C)(C)C*	11	12	5
Napthenics (cyclic)	C1CCC(CCC)CC1	84	88	40
	C1C(C)CC(C)C(C)C1	104	109	49

	C1CC2CCCCC2CC1	100	104	47
	C1C(CCC)CC(CC)CC1	22	22	10
	C1CC(C(C)C)CCC1(C(C)C)	16	16	7

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

A semi-static 21-day reproduction test was conducted by EMBSI (2004) with *Daphnia magna* for Isopar G and H, respectively. Exposure concentrations were produced with a gas saturation method and the exposure medium was changed daily (daphnids moved to fresh media). Ten test replicates (1 daphnid in each flask) were run for each exposure level in closed flasks of 125 ml without headspace. Nominal test concentrations were 0, 26 and 85 µg l^{-1} for Isopar G and 0, 20 and 40 µg l^{-1} for Isopar H (control shared with Isopar G). The actual exposure concentrations were based on geometric means of measured concentrations (equipment: HS GC-FID) of fresh and old media of days 0-1, 7-8, 14-15 and 20-21 were 0, 25 and 50 µg l^{-1} for Isopar G and 0, 11 and 15 µg l^{-1} for Isopar H. Hardness, pH, dissolved oxygen and temperature of the test media were in the limits required by present test standards. Results of the study are provided in the following table.

Table 6.1 Results of the long-term test with Daphnia magna (EMBSI, 2004).

Exposure level	Immobilisation (%)	Average number of neonatates per survived adult at the end of the experiment	Adult average length (mm)
0	0*	119*	4.6
25 µg l^{-1} Isopar G	0	119	4.4
50 µg l^{-1} Isopar G	100 (at 48 h)	n/a	n/a
11 µg l^{-1} Isopar H	0**	125**	4.5
15 µg l^{-1} Isopar H	100 (at day 9)	n/a	n/a

*One daphnid damaged by a broken transfer pipette used on day 14; death on day 15. Neonatates of this adult were not included in the calculation of the average number of neonatates.

**Four daphnids damaged (not swimming properly) by a broken transfer pipette used on day 14. Deaths of the damaged daphnids followed on days 15 and 16. Neonatates of these adults were not included in the calculation of the average number of neonatates.

A NOEC of 11 µg l^{-1} for Isopar H and a NOEC of 25 µg l^{-1} for Isopar G based on measured concentrations can be derived for all three endpoints from this well documented limit test, although it must be noted, that the amount of replicates was the minimum required by present standards.

A similar semi-static 21-day test with *Daphnia magna* has also been conducted for test substance corresponding with the identity of hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated (CAS 93685-81-5) and containing mainly pentamethylheptanes (C12). A NOEC of 13 µg l^{-1} was obtained in the study. For further details, see PBT summary no. 62.

6.1.1.3 Algae and aquatic plants

A static ecotoxicity test with *Scenedesmus subspicatus* is available for test substance corresponding with the identity of hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated (CAS 93685-81-5) and containing mainly pentamethylheptanes (C12). For further details, see PBT summary no. 62.

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: Alkanes, C9-12-iso- do not meet the P/vP criteria based on screening data. Standard ready biodegradation test results are available for two products Isopar G and Isopar H and they indicate, that these multi-constituent substances are not readily biodegradable. However, some biodegradation was observed in the tests. No inherent biodegradation or simulation test data are available for these substances. According to QSAR -predictions (including BIOWIN2 and 3) for selected typical and realistic worst case (C9-C12 and cyclic) constituents with a degree of branching between 2 and 4, these constituents are considered as not persistent. CATABOL predicts, that all

constituents are biodegraded through the same metabolic pathway to corresponding alcohols and further to acids. An assessment of penta-branched alkanes, which may be present in the substance, has been presented in PBT summary no. 62 (P/vP criteria fulfilled based on screening data, but overall conclusion “not PBT”).

Bioaccumulation: Based on QSAR-predictions of logKow –values and BCF of selected 2 to 4 branched alkanes, it is considered, that some of the constituents may fulfil the B criterion based on screening data. The biodegradation products (corresponding alcohols and acids) of the constituents are not expected to have relevant bioaccumulation potential. For penta-branched alkanes a conclusion “not fulfilling the B criterion as borderline case” was drawn (see PBT summary no. 62). It is noted, that no final conclusion was derived for the substance by the PBT subgroup regarding its bioaccumulation potential.

Toxicity: Looking solely at logKow –values of the constituents and assuming baseline toxicity, it could be expected, that C12-isoalkanes with < 5 branches exhibit a slightly higher toxicity than pentamethylheptanes. The substance containing mainly pentamethylheptanes (see PBT summary no. 62) was concluded based on a long-term daphnia test and an acute algae test to be not T as borderline case. Experimental 21d-NOECs of 11 µg l^{-1} and 25 µg l^{-1} were determined for Isopar Isopar H and G. QSAR-predictions for the ecotoxicity of selected 2 to 4 branched alkanes indicate, that the T criterion would not be fulfilled as borderline case. It is, however, noted, that no final conclusion regarding T-criterion was drawn by the PBT subgroup.

Summary: Alkanes, C9-12-iso- is an UVCB substance. Its 2- to 4 branched possible consituents are considered not to fulfil the P/vP –criteria based on screening data. The predicted biodegradation products are not expected to have relevant bioaccumulation potential. No final conclusion was drawn regarding B and T criteria for the parent compound. The potential penta-branched constituents are not considered as PBT (see PBT summary no. 62) . It is concluded, that alkanes, C9-12-iso- 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:

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Other sources:

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