REPUBLIKA SLOVENIJA
MINISTRSTVO ZA ZDRAVJE
URAD REPUBLIKE SLOVENIJE ZA KEMIKALIJE

SUBSTANCE EVALUATION CONCLUSION

as required by REACH Article 48

and

EVALUATION REPORT

for

Reaction mass of 2-methylpent-2-ene and diisopropylether

EC No 906-484-8

CAS No not applicable

Evaluating Member State(s): Slovenia

Dated: October 2016

Evaluating Member State Competent Authority

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Year of evaluation in CoRAP: 2015

Member State concluded the evaluation without any further need to ask more information from the registrants under Article 46(1) decision.

Further information on registered substances here:

http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances

DISCLAIMER

This document has been prepared by the evaluating Member State as a part of the substance evaluation process under the REACH Regulation (EC) No 1907/2006. The information and views set out in this document are those of the author and do not necessarily reflect the position or opinion of the European Chemicals Agency or other Member States. The Agency does not guarantee the accuracy of the information included in the document. Neither the Agency nor the evaluating Member State nor any person acting on either of their behalves may be held liable for the use which may be made of the information contained therein. Statements made or information contained in the document are without prejudice to any further regulatory work that the Agency or Member States may initiate at a later stage.

Foreword

Substance evaluation is an evaluation process under REACH Regulation (EC) No. 1907/2006. Under this process the Member States perform the evaluation and ECHA secretariat coordinates the work. The Community rolling action plan (CoRAP) of substances subject to evaluation, is updated and published annually on the ECHA web site[1].

Substance evaluation is a concern driven process, which aims to clarify whether a substance constitutes a risk to human health or the environment. Member States evaluate assigned substances in the CoRAP with the objective to clarify the potential concern and, if necessary, to request further information from the registrant(s) concerning the substance. If the evaluating Member State concludes that no further information needs to be requested, the substance evaluation is completed. If additional information is required, this is sought by the evaluating Member State. The evaluating Member State then draws conclusions on how to use the existing and obtained information for the safe use of the substance.

This Conclusion document, as required by Article 48 of the REACH Regulation, provides the final outcome of the Substance Evaluation carried out by the evaluating Member State. The document consists of two parts i.e. A) the conclusion and B) the evaluation report. In the conclusion part A, the evaluating Member State considers how the information on the substance can be used for the purposes of regulatory risk management such as identification of substances of very high concern (SVHC), restriction and/or classification and labelling. In the evaluation report part B the document provides explanation how the evaluating Member State assessed and drew the conclusions from the information available.

With this Conclusion document the substance evaluation process is finished and the Commission, the Registrant(s) of the substance and the Competent Authorities of the other Member States are informed of the considerations of the evaluating Member State. In case the evaluating Member State proposes further regulatory risk management measures, this document shall not be considered initiating those other measures or processes. Further analyses may need to be performed which may change the proposed regulatory measures in this document. Since this document only reflects the views of the evaluating Member State, it does not preclude other Member States or the European Commission from initiating regulatory risk management measures which they deem appropriate.

[1] http://echa.europa.eu/regulations/reach/evaluation/substance-evaluation/community-rolling-action-plan

Contents

Part A. Conclusion

1. CONCERN(S) SUBJECT TO EVALUATION

Reaction mass of 2-methylpent-2-ene and diisopropyl ether (EC No 906-484-8) was originally selected for substance evaluation in order to clarify concerns about:

- Suspected PBT/vPvB (The substance (reaction mass) contains diisopropyl ether and 2-methylpent-2-ene and various identified impurities with up to < 10 % in concentration. One theoretical constituent A, which is used as a worst-case representative structure for unidentified low concentration (i.e. < 1 %) constituents in the substance, is suspected to have PBT properties);
- Exposure of environment/Wide dispersive use, high tonnage

2. OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

Not applicable

3. CONCLUSION OF SUBSTANCE EVALUATION

The evaluation of the available information on the substance has led the evaluating Member State to the following conclusions, as summarised in the table below.

Table 1

CONCLUSION OF SUBSTANCE EVALUATION Conclusions	Tick box
Need for follow-up regulatory action at EU level	
Harmonised Classification and Labelling	
Identification as SVHC (authorisation)	
Restrictions	
Other EU-wide measures	
No need for regulatory follow-up action at EU level	X

4. FOLLOW-UP AT EU LEVEL

4.1. Need for follow-up regulatory action at EU level

4.1.1. Harmonised Classification and Labelling

Not applicable.

4.1.2. Identification as a substance of very high concern, SVHC (first step towards authorisation)

Not applicable.

4.1.3. Restriction

Not applicable.

4.1.4. Other EU-wide regulatory risk management measures

Not applicable.

5. CURRENTLY NO FOLLOW-UP FORESEEN AT EU LEVEL

5.1. No need for regulatory follow-up at EU level

Table 2

REASON FOR REMOVED CONCERN The concern could be removed because	Tick box
Clarification of hazard properties/exposure	X
Actions by the registrants to ensure safety, as reflected in the registration dossiers (e.g. change in supported uses, applied risk management measures, etc.)	

Taking into consideration the PBT and vPvB criteria detailed in Annex XIII of REACH, the information submitted by the Registrant and based on expert judgment, Reaction mass of 2-methylpent-2-ene and diisopropylether does not meet the criteria for bioaccumulation (B or vB).

5.2. Other actions

No need for other follow-up actions based on this substance evaluation.

6. TENTATIVE PLAN FOR FOLLOW-UP ACTIONS (IF NECESSARY)

Not applicable.

Part B. Substance evaluation

7. EVALUATION REPORT

According to Article 45(4) of the REACH Regulation the Competent Authority of Slovenia has initiated substance evaluation of Reaction mass of 2-methylpent-2-ene and diisopropyl ether (EC No 906-484-8), based on a registration submitted by the registrant and prepared the decision in accordance with Article 46(1) of the REACH Regulation.

7.1. Overview of the substance evaluation performed

EC No 906-484-8 was originally selected for substance evaluation in order to clarify concerns about:

-The substance (reaction mass) contains diisopropyl ether and 2-methylpent-2-ene and various identified impurities with up to < 10 % in concentration. One theoretical constituent A, which is used as a worst-case representative structure for unidentified low concentration (i.e. < 1 %) constituents in the substance, is suspected to have PBT properties.

Table 3

EVALUATED ENDPOINTS	
Endpoint evaluated	**Outcome/conclusion**
PBT/vPvB	Based on the evaluation the eMSCA concludes that the substance or its constituents do not meet the criteria for bioaccumulation (B or vB).

7.2. Procedure

On the basis of an opinion of the ECHA Member State Committee and due to initial grounds for concern relating to possible PBT/vPvB properties Reaction mass of 2-methylpent-2-ene and diisopropylether was included in the Community rolling action plan (CoRAP) for substance evaluation according to Article 44(2) of the REACH Regulation to be evaluated in 2015. The CoRAP was published on the ECHA website on 17 March 2015 and the Competent Authority of Slovenia was appointed as the evaluating Member State Competent Authority (eMSCA).

According to Article 45(4) of the REACH Regulation the Competent Authority of Slovenia has initiated substance evaluation of Reaction mass of 2-methylpent-2-ene and diisopropyl ether (EC No 906-484-8), based on a registration submitted by the registrant.

The eMSCA consulted with PBT Expert Group regarding the evaluation of PBT properties for Reaction mass of 2-methylpent-2-ene and diisopropyl ether. The eMSCA decided not to ask further information from the registrant in a decision in accordance with Article 46(1) of the REACH Regulation and concluded the case.

7.3. Identity of the substance

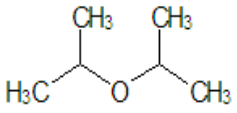
Based on the available information, the substance is confirmed as an UVCB substance, because the ratio between constituents is variable and poorly predictable.

Table 4

SUBSTANCE IDENTITY	
Public name:	Reaction mass of 2-methylpent-2-ene and diisopropyl ether
EC number:	EC No 906-484-8
CAS number:	Not applicable
Index number in Annex VI of the CLP Regulation:	-
Molecular formula:	Not applicable as multiconstituent substance.
Molecular weight range:	Not applicable as multiconstituent substance.
Synonyms:	OC4 Produktstrom 7 reaction mass of DIPE and 2-methylpent-2-ene

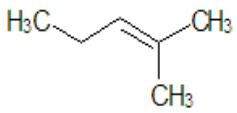
Type of substance ☐ Mono-constituent ☐ Multi-constituent ☒ UVCB

Structural formula:



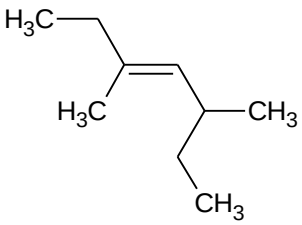
CC(C)OC(C)C

Diisopropylether



C/C(C)=C\CC

2-Methyl-2-penten



3,5-dimethylhept-3-ene

Worst-case theoretical constituent A, used for PBT assessment = 3,5-dimethylhept-3-ene; CAS 59643-68-4

The information on composition is in line with the analytical methods provided by Registrant. For identification of Registrant substance following methods were used and described: Ultraviolet-Visible Spectroscopy (UV-VIS), Infrared Spectroscopy (IR), Proton-Nuclear Magnetic resonance spectroscopy (1H NMR), Carbon Nuclear Magnetic resonance spectroscopy (13C NMR) and Gas Chromatography – Mass Spectroscopy (GC-MS). The substance is confirmed as a substance of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB) - substances for which the number of constituents is high, or the composition is to a significant extent unknown, or the variability of composition is large or unpredictable.

UVCB substance

Table 5

Major constituents	Typical concentration	Concentration range	Remarks
diisopropylether (DIPE) EC no: 203-560-6	Confidential	Confidential	
2-methylpent-2-ene EC no: 210-883-6	Confidential	Confidential	

Table 6

Minor constituent	Typical concentration	Concentration range	Remarks
3,5-dimethylhept-3-ene = constituent A	<1.0 % (w/w)	<1.0 % (w/w)	theoretical constituent used as representative structure for unidentified low concentration (i.e. < 1 %) constituents in the substance

7.4. Physico-chemical properties

Table 7

OVERVIEW OF PHYSICOCHEMICAL PROPERTIES – REGISTERED SUBSTANCE[2]	
Property	**Value**
Physical state at 20°C and 101.3 kPa	Yellow liquid
Vapour pressure	12794 Pa at 20 °C and 15519 Pa at 25 °C
Water solubility	2.828 ± 0.405 g/L at 20 ± 0.5 °C
Partition coefficient n-octanol/water (Log Kow)	range 2.357 – 4.255 for the main components with an estimated overall range of 0 - 4.3 including hydrophilic impurities
Flammability	highly flammable
Explosive properties	not explosive
Dissociation constant	not relevant for ethers and branched alkenes
Relative density	0.7165 g/cm^3 at 20 °C
OVERVIEW OF PHYSICOCHEMICAL PROPERTIES – THEORETICAL CONSTITUENT A	
Property	**Value**
Vapour pressure	16500 Pa at 25 °C (Mean VP of Antoine & Grain methods, EPISUITE)
Water solubility	3.744 mg/L at 25 °C (WSKOW v1.42)
Partition coefficient n-octanol/water (Log Kow)	4.53 (KOWWIN v1.68 estimate)

7.5. Manufacture and uses

7.5.1. Quantities

Tonnage band: 1000-10 000 tonnes per annum.

[2] Based on data from the registration dossier

7.5.2. Overview of uses

The registered substance is used as a fuel additive.

Table 8

USES Use(s)	
Manufacture	IU1 - Manufacture of Substance
Uses at industrial sites	IU2 - Distribution of the substance IU3 - Use as fuel - Industrial
Uses by professional workers	IU4 - Use as fuel - Professional
Consumer Uses	IU5 - Use as fuel - Consumer

7.6. Classification and Labelling

7.6.1. Harmonised Classification (Annex VI of CLP)

No harmonized classification available.

7.6.2. Self-classification

In the registration*:*

Flam. Liquid 2 H225: Highly flammable liquid and vapour.
Asp. Tox. 1 H304: May be fatal if swallowed and enters airways.
STOT Single Exp. 3 H336: May cause drowsiness or dizziness.
Affected organs: Central nervous system (narcotic effect), Inhalation
Aquatic Chronic 2 H411: Toxic to aquatic life with long lasting effects.

7.7. Environmental fate properties

7.7.1. Degradation

EC No 906-484-8

There is a ready biodegradability test available for the whole substance EC No 906-484-8. The results are reported below and indicate that the substance is not readily biodegradable. The P screening criterion is therefore met for the registered substance. This study is not considered as sufficient for the PBT assessment, for which 3,5-dimethylhept-3-ene is used as representative structure.

Method	Results	Remarks
Test type: ready biodegradability activated sludge, domestic, non-adapted ISO Guideline 14593: "Water quality - Evaluation of ultimate aerobic biode-gradability of organic compounds in aqueous medium – Method by analysis of inorganic carbon in sealed vessels (CO2 headspace test)" OECD Guideline 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)	not readily biodegradable% Degradation of test substance: 3.6 after 0 d (CO_2 evolution) (Based on 2 replicates) 5 after 5 d (CO_2 evolution) (Based on 2 replicates) 6 after 13 d (CO_2 evolution) (Based on 2 replicates) 3.8 after 21 d (CO_2 evolution) (Based on 2 replicates) 19.5 after 28 d (CO_2 evolution) (Based on 2 replicates)	1 (reliable without restriction) key study experimental result **Test material:** reaction mass of 2-methylpent-2-ene and diisopropyl ether

QSAR predictions of biodegradation have been performed for the starting materials and theoretical constituent A:

diisopropylether

BIOWIN v4.10 provides for diisopropylether the following biodegradation predictions:

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 0.3649
Biowin2 (Non-Linear Model): 0.1864
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.0267 (weeks)
Biowin4 (Primary Survey Model): 3.7311 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): 0.5927
Biowin6 (MITI Non-Linear Model): 0.7643
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.4717
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation model

2-methylpent-2-ene

BIOWIN v4.10 provides for 2-methylpent-2-ene the following biodegradation predictions:

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 0.7075
Biowin2 (Non-Linear Model): 0.8598
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.0132 (weeks)
Biowin4 (Primary Survey Model): 3.7263 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): 0.5186
Biowin6 (MITI Non-Linear Model): 0.6485
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.5498
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
LOG BioHC Half-Life (days): 0.2589
BioHC Half-Life (days): 1.8150

Theoretical constituent A: 3,5-dimethylhept-3-ene

3,5-dimethylhept-3-ene does not contain functional groups that are easily hydrolyzed. Consequently, 3,5-dimethylhept-3-ene is considered as resistant to hydrolysis and hydrolysis will not contribute to the degradation of the substance in the environment.

No tests are available for 3,5-dimethylhept-3-ene. BIOWIN v4.10 provides for 3,5-dimethylhept-3-ene the following biodegradation predictions:

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 0.6874
Biowin2 (Non-Linear Model): 0.7714
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.9202 (weeks)
Biowin4 (Primary Survey Model): 3.6656 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): 0.3926
Biowin6 (MITI Non-Linear Model): 0.4370
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.3304
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
LOG BioHC Half-Life (days): 0.5194

Concerning **phototransformation in air**, 3,5-dimethylhept-3-ene has the potential to volatilize to air based on a high vapour pressure where it is subject to atmospheric oxidation by means of hydroxyl radicals (OH-). The estimated Half-life (DT_{50}) for 3,5-dimethylhept-3-ene is 0.116 days at 25°C based on assumption of 12-hour day (AOPWIN v1.92). Thus, 3,5-dimethylhept-3-ene is expected to rapidly degrade in the atmosphere by hydroxyl radical attack based on QSAR estimations of atmospheric half-lives.

Data on phototransformation in water or soil are not available.

In conclusion, diisopropylether and 2-methylpent-2-ene are based on BIOWIN v4.10 QSAR estimates predicted to be readily biodegradable, whereas theoretical worst-case constituent 3,5-dimethylhept-3-ene is predicted to be not readily biodegradable.

7.7.2. Environmental distribution

EC No 906-484-8

There is an adsorption test according to HPLC method available for the whole substance EC No 906-484-8. The results for the study on the whole substance are as follows:

Method	Results	Remarks
Study type: adsorption (soil/sewage sludge) HPLC estimation method OECD Guideline 121: "Estimation of the Adsorption Coefficient (Koc) on Soil and on Sewage Sludge using High Performance Liquid Chromatography (HPLC))" EU Method C.19 (Estimation of the Adsorption Coefficient (Koc) on Soil and on Sewage Sludge using High Performance Liquid Chromatography (HPLC))	Adsorption coefficient: log Koc: 1.412 – 2.559 at 25°C (mean of 3 replicates)	1 (reliable without restriction) key study experimental result Test material: (EC name) Reaction mass of 2-methylpent-2-ene and diisopropyl ether

This study is not considered as sufficient for the PBT assessment, for which 3,5-dimethylhept-3-ene is used as representative structure.

Theoretical constituent A: 3,5-dimethylhept-3-ene:

No tests are available for 3,5-dimethylhept-3-ene. EPI Suite provides for 3,5-dimethylhept-3-ene the following QSAR predictions:

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc: 589.4 L/kg (MCI method)
Log Koc: 2.770 (MCI method)
Koc: 8535 L/kg (Kow method)
Log Koc: 3.931 (Kow method)

In conclusion, the registered substance has a low potential for adsorption to soil and sediment whereas theoretical constituent A is predicted to have a higher potential for adsorption.

7.7.3. Bioaccumulation

EC No 906-484-8

No data for the whole substance available. The measured Log Kow is 2.357-4.255 which is below the threshold of 4.5 for screening as potentially B or vB. However, this is not considered as sufficient for the PBT assessment, for which 3,5-dimethylhept-3-ene is used as representative structure.

QSAR predictions of biodegradation have been performed for the starting materials and theoretical constituent A:

diisopropylether

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
Log Biotransformation Half-life (HL) = -0.9383 days (HL = 0.1153 days)
Log BCF Arnot-Gobas method (upper trophic) = 0.211 (BCF = 1.625)
Log BAF Arnot-Gobas method (upper trophic) = 0.211 (BAF = 1.625)
log Kow used: 0.89 (expkow database)

2-methylpent-2-ene

Bioaccumulation Estimates (BCFBAF v3.01) for 2-methylpent-2-ene:
Log BCF from regression-based method = 1.732 (BCF = 53.91 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 0.0672 days (HL = 1.167 days)
Log BCF Arnot-Gobas method (upper trophic) = 2.043 (BCF = 110.5)
Log BAF Arnot-Gobas method (upper trophic) = 2.043 (BAF = 110.5)
log Kow used: 3.13 (estimated)

Theoretical constituent A: 3,5-dimethylhept-3-ene

No empirical bioconcentration, bioaccumulation or K_{OW} data are available for 3,5-dimethylhept-3-ene. QSAR estimated log Kow of 3,5-dimethylhept-3-ene is 4.53 (EPI Suite).

Bioaccumulation Estimates (BCFBAF v3.01) for 3,5-dimethylhept-3-ene :
Log BCF from regression-based method = 2.655 (BCF = 452.1 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 0.4676 days (HL = 2.935 days)
Log BCF Arnot-Gobas method (upper trophic) = 2.954 (BCF = 898.7)
Log BAF Arnot-Gobas method (upper trophic) = 2.960 (BAF = 911.7)
log Kow used: 4.53 (estimated)

In conclusion, the screening criterion for B/vB is met for 3,5-dimethylhept-3-ene based on its predicted Log Kow.

7.8. Environmental hazard assessment

7.8.1. Aquatic compartment (including sediment)

7.8.1.1. Fish

EC No 906-484-8

There is an acute fish toxicity test available for the whole substance EC No 906-484-8.

Method	Results	Remarks
Brachydanio rerio (new name: *Danio rerio*) OECD Guideline 203: Fish, Acute Toxicity Test EU Method C.1 (Ac ute Toxicity for Fish)	LC_{50} (24 h): > 10 mg/L diss. (diss. org. carbon) (geom. mean meas.) LC_{50} (48 h): > 10 mg/L diss. diss. org. carbon) (geom. mean meas.) LC_{50} (72 h): > 10 mg/L diss. (diss. org. carbon) (geom. mean meas.) LC_{50} (96 h): > 10 mg/L diss. (diss. org. carbon) (geom. mean meas.)	1 (reliable without restriction) key study experimental result Test material: (EC name) Reaction mass of 2-methylpent-2-ene and diisopropyl ether

This study is not considered as sufficient for the PBT assessment, for which 3,5-dimethylhept-3-ene is used as representative structure.

Theoretical constituent A: 3,5-dimethylhept-3-ene

No tests are available for 3,5-dimethylhept-3-ene. Due to the high volatility of 3,5-dimethylhept-3-ene (estimated Henry Law Constant 1.18E+5 Pa m^3 $mole^{-1}$) reliable testing of its toxicity to fish would be difficult and would need to be supported by adequate analytical measurements. The QSAR predicted 96-h LC_{50} for fish is 0.555 mg/L (ECOSAR v11).

7.8.1.2. Aquatic invertebrates

EC No 906-484-8

There is an acute Daphnia toxicity test available for the whole substance EC No 906-484-8.

Method	Results	Remarks
Daphnia magna, freshwater, static OECD Guideline 202 (Daphnia sp. Acute Immobilisation Test) EU Method C.2 (Acute Toxicity for Daphnia) ISO 6341 15 (Water quality – Determination of the Inhibition of the Mobility of Daphnia magna Straus (Cldocera, Crustacea)	EC_{50} (24 h): 19 mg/L diss. (diss. org. carbon) (geom. mean meas.) based on immobilisation EC_{50} (48 h): 6.9 mg/L diss. (diss. org. carbon) (geom. mean meas.) based on immobilisation	1 (reliable without restriction) key study experimental result Test material: (EC name) Reaction mass of 2-methylpent-2-ene and diisopropyl ether

This study is not considered as sufficient for the PBT assessment, for which 3,5-dimethylhept-3-ene is used as representative structure.

Theoretical constituent A: 3,5-dimethylhept-3-ene

No tests are available for 3,5-dimethylhept-3-ene. Due to the high volatility of 3,5-dimethylhept-3-ene (estimated Henry Law Constant 1.18E+5 Pa m^3 $mole^{-1}$) reliable testing of its toxicity to Daphnia would be difficult and needs to be supported by adequate analytical measurements. The QSAR predicted 48-h EC_{50} for daphnids is 0.396 mg/L (ECOSAR v11).

7.8.1.3. Algae and aquatic plants

EC No 906-484-8
There is an algal growth inhibition test available for the whole substance EC No 906-484-8.

Method	Results	Remarks
Desmodesmus subspicatus, freshwater, static OECD Guideline 201 (Alga, Growth Inhibition Test) EU Method C.3 (Algal Inhibition Test)	EC_{50} (72 h): 22 mg/L diss. (diss. org. carbon) (geom. mean meas.) based on growth rate EC_{50} (72 h): 6.6 mg/L diss. (diss. org. carbon) (geom. mean meas.) based on biomass EC_{50} (72 h): 4.2 mg/L diss. (diss. org. carbon) (geom. mean meas.) based on yield	1 (reliable without restriction) key study experimental result Test material: (EC name) Reaction mass of 2-methylpent-2-ene and diisopropyl ether

This study is not considered as sufficient for the PBT assessment, for which 3,5-dimethylhept-3-ene is used as representative structure.

Theoretical constituent A: 3,5-dimethylhept-3-ene

No tests are available for 3,5-dimethylhept-3-ene. Due to the high volatility of 3,5-dimethylhept-3-ene (estimated Henry Law Constant 1.18E+5 Pa m^3 $mole^{-1}$) reliable testing of its effects on algae would be difficult and needs to be supported by adequate analytical measurements. The QSAR predicted 96-h EC50 for green algae is 0.449 mg/L (ECOSAR v11).

7.8.1.4. Sediment organisms

No tests are available for 3,5-dimethylhept-3-ene or for the whole substance EC No 906-484-8.

7.8.1.5. Other aquatic organisms

No data available.

7.8.2. Terrestrial compartment

No tests are available for 3,5-dimethylhept-3-ene or for the whole substance EC No 906-484-8.

7.8.3. Microbiological activity in sewage treatment systems

EC No 906-484-8
There is an activated sludge respiration inhibition test available for the whole substance EC No 906-484-8:

Method	Results	Remarks
activated sludge of a predominantly domestic sewage, freshwater, static OECD Guideline 209 (Activated Sludge, Respiration Inhibition Test) EU Method C.11 (Biodegradation, Activated Sludge Respiration Inhibition Test)	NOEC (3 h):10 mg/L test mat. (nominal) based on respiration rate EC_{50} (3 h): 3000 mg/L test mat. (nominal) based on respiration rate	1 (reliable without restriction) key study experimental result Test material: (EC name) Reaction mass of 2-methylpent-2-ene and diisopropyl ether

Theoretical constituent A: 3,5-dimethylhept-3-ene

No tests are available for 3,5-dimethylhept-3-ene. Due to the high volatility of 3,5-dimethylhept-3-ene (estimated Henry Law Constant 1.18E+5 Pam^3 $mole^{-1}$) reliable testing of its effects on activated sludge respiration would be difficult and would need to be supported by adequate analytical measurements.

7.8.4. PNEC derivation and other hazard conclusions

Not evaluated.

7.8.5. Conclusions for classification and labelling

Not evaluated.

7.9. Human Health hazard assessment

Assessment of human health endpoints including hazard assessment of physical-chemical properties was not in the scope of eMSCA evaluation.

7.10. Assessment of endocrine disrupting (ED) properties

Assessment of endocrine disrupting properties was not in the scope of eMSCA evaluation.

7.11. PBT and VPVB assessment

The registered substance is a UVCB. The PBT assessment was performed on theoretical constituent A, 3,5-dimethylhept-3-ene. 3,5-dimethylhept-3-ene was suspected to have PBT properties and was selected as the representative worst-case structure for PBT assessment.

In order to support the PBT assessment, data from structurally-related alkanes and alkenes is used as described in Tables 9 and 10.

Table 9: Data from structurally related Alkanes used in support of the PBT assessment

Name	2,2,4,6,6-pentamethylheptane[1]	Alkanes, C9-12-iso-[1]	2,3 dimethylheptane[1]	dimethyldecane[1]
CAS No	13475-82-6	90266-57-4	3074-71-3	-
EC No	236-757-0	292-459-0	679-707-7	-
Molecular weight	170.33	Not applicable, UVCB	128.26	-
Structural formula	C12H26 	Not applicable, UVCB	C9H20 CC(C)(C)CCCCC	-
Physical state at room temperature	Liquid	Liquid	Liquid	-
Vapour pressure/unit	1 hPa (at 20°C)*	0.66 hPa (at 20 °C) 1.8 hPa (at 20 °C)	-	-
Water solubility/unit	0.151 mg/L (at 25°C)**	Not applicable	3.11 mg/L (at 25°C)	-
Log Kow	6.4 (CLOGP)*** 5.94 (KOWWIN v1.67)	Not applicable	4.61 (KOWWIN v1.67)	-
Log Koc	-	-	2.779 (KOCWIN)	-
BCF	888 1341 (dietary)	C9: 712-760 C10: 539-574 C11: 1056-1371 C12: 2689-3072 (BCFWIN V2.16)	713 (QSAR) 1842 (exp. dietary)	9715 (QSAR) 2500 (exp. dietary)[2]
Hydrolytic stability	-	-	-	-
Biodegradation	Not readily biodegradable (BIOWIN v4.02)	Not readily biodegradable	Not readily biodegradable (BIOWIN v4.10)	
Short-term toxicity to fish LC_{50} (96 h) [mg/L]	0.009 QSAR (ECOSAR v0.99h)	C9: 0.024-0.046 C10: 0.015-0.022	0.473 (ECOSAR v11)	-

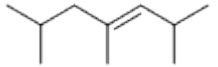
		C11: 0.011-0.017 C12: 0.011-0.012 Narcosis Target Lipid Model of McGrath et al. (2004)		
Short-term toxicity to aquatic invertebrates D. magna EC_{50} (48 h) [mg/L]	0.013 QSAR (ECOSAR v0.99h)	C9: 0.025-0.048 C10: 0.015-0.023 C11: 0.012-0.018 C12: 0.011-0.013 Narcosis Target Lipid Model of McGrath et al. (2004)	0.340 (ECOSAR v11)	-
Reproduction toxicity to daphnids NOEC (21 d) [mg/L]	0.013 (exp. OECD 211)	-	-	-
Toxicity to aquatic algae and cyano-bacteria ErC50 (72 h) [mg/L]	0.011 QSAR (ECOSAR v0.99h)	C11: 0.005-0.008 C12: 0.005-0.006 Narcosis Target Lipid Model of McGrath et al. (2004)	0.387 (ECOSAR v11)	-

[1] PBT Working Group (2008). ECB Summary factsheet PBT LIST No. 24 Alkanes, C9-12-iso-. Available at: http://echa.europa.eu/documents/10162/264bfee3-eff2-4119-9668-e7c5f703ab1d
[2] Reference to Parkerton T., Letkinski, D., Febbo, E., Davi, R., Dzamba, C., Connelly, M., Christensen, K. And Peterson, D., 2001. A practical testing approach for assessing bioaccumulation potential of poorly water soluble organic chemicals. Presentation at SETAC Europe, Madrid. There are several isomers, but no specific information on substance identity is provided.
* VP 1 hPa at 25°C according to registration dossier as available on ECHA's website
** Water solubility 4.86 µg/L according to registration dossier as available on ECHA's website
*** Log Kow 6.96 according to registration dossier as available on ECHA's website

Table 10: Data from structurally related Alkenes used in support of the PBT assessment

(c) calculated data

(m) measured data

Name	2-hexene	2-heptene	2-octene	2-nonene	2,4,6-trimethylhept-3-ene
CAS No	25264-93-1	25339-56-4	25377-83-7	27215-95-8	126690-66-2
EC No	203-777-6	246-871-2	246-920-8	248-339-5	-
Molecular weight	86.18	98.19	121.21	126.24	140.27
Structural formula	CH3-CH=CH-(CH2)2-CH3	CH3-CH=CH-(CH2)3-CH3	CH3-CH=CH-(CH2)4-CH3	CH3-CH=CH-(CH2)5-CH3	
Physical state at room temperature	Colorless liquid	Colorless liquid	Colorless liquid	Colorless liquid	-
Vapour pressure/unit	230.6 hPa at 25°C (m and c) [1]	74.66 hPa at 25°C (c) [1] 79.05 hPa at 25°C [1-heptene] (m) [1]	22 hPa at 25°C (c) [1] 23.2 hPa at 25°C [1-octene] (m) [1]	5.00 hPa at 25°C (m) [1]	11200 Pa at 25 °C (Mean VP of Antoine & Grain methods, EPISUITE)
Water solubility/unit	50 mg/L at 20°C [1]	13.45 mg/l at 25°C (c) [1] 18.2 mg/l at 25°C [1-heptene] (m) [1]	3.65 mg/l at 25°C (c) [1] 4.1 mg/l at 25°C [1-octene] (m) [1]	3.619 mg/l at 25°C (c)[1]	1.447 mg/L at 25 °C (WSKOW v1.42, EPISUITE)
Log Kow	3.07 (c) [1] 3.39 at 25° C [1-hexene](m)	3.64 (c) [1] 3.99 [1-heptene] (m) [1]	4.13 (c) [1] 4.57 [1-octene](m) [1]	4.55 (c) [1]	4.95 (KOWWIN v1.68, EPISUITE)
Log Koc	2.66 (KOCWIN) [1]	3.09 (KOCWIN) [1]	3.91 (KOCWIN) [1]	3.95 (KOCWIN) [1]	4.296 (Kow method, EPISUITE)
BCF	46 L/kg (EPIWIN Suite) [1]	236 L/kg (EPIWIN Suite) [1]	659 L/kg (EPIWIN Suite) [1]	632 L/kg (EPIWIN Suite) [1]	852.6 L/kg (BCFBAF V3.01 regression based method, EPISUITE) 2354 L/kg (BCFBAF V3.01 Arnot-Gobas method, EPISUITE) 1950 L/kg (m) [2]
Hydrolytic stability	stable [1]	stable [1]	stable [1]	stable [1]	-
Biodegradation	77% at 28 days (OECD	BIOWIN 3: 3.2804 (days-	BIOWIN 3: 3.5497 (days-	BIOWIN 3: 3.5169 (days-	BIOWIN 3: 2.8892 (weeks)

	301C) 22% at 28 days (Closed Sturm) BIOWIN 3: 3.3115 (days-weeks) BIOWIN 4: 3.9954 (days) BIOWIN 5: 0.5738 BIOWIN 6: 0.7409 Ready biodegr.pred. YES (EPISUITE)	weeks) BIOWIN 4: 3.9751 (days) BIOWIN 5: 0.5815 BIOWIN 6: 0.7456 Ready biodegr.pred. YES (EPISUITE)	weeks) BIOWIN 4: 4.2240 (days) BIOWIN 5: 0.5892 BIOWIN 6: 0.7503 Ready biodegr.pred. YES (EPISUITE)	weeks) BIOWIN 4: 4.2037 (days) BIOWIN 5: 0.5968 BIOWIN 6: 0.7548 Ready biodegr.pred. YES (EPISUITE)	BIOWIN 4: 3.6454 (days-weeks) BIOWIN 5: 0.2512 BIOWIN 6: 0.2372 Ready biodegr.pred. NO (EPISUITE)
Short-term toxicity to fish LC_{50} (96 h) [mg/L]	6.16 (ECOSAR) 5.6 [1-heptene] (m) [1]	2.09 (ECOSAR)	0.83 (ECOSAR)	0.38 (ECOSAR)	0.260 (ECOSAR)
Short-term toxicity to aquatic invertebrates *D. magna* EC_{50} (48 h) [mg/L]	7.10 (ECOSAR) 32 (m, estimated) [1]	2.51 (ECOSAR)	1.03 (ECOSAR)	0.48 (ECOSAR)	0.193 (ECOSAR)
Toxicity to aquatic algae and cyano-bacteria ErC_{50} (72 h) [mg/L]	4.72 (ECOSAR) >solubility (m) [1]	1.73 (ECOSAR)	0.73 (ECOSAR)	0.35 (ECOSAR)	0.227 (ECOSAR)

[1] OECD (2010): OECD SIDS C7-C9 Aliphatic Hydrocarbon Solvents Category Assessment Report. Available at: http://webnet.oecd.org/HPV/UI/Search.aspx
[2] Dimitrov et al. (2005). Base-line model for identifying the bioaccumulation potential of chemicals. SAR and QSAR in Environmental Research, Volume 16, Issue 6, 2005, 531-554

Persistence assessment

Experimental data on **biodegradation in water or soil** are not available for 3,5-dimethylhept-3-ene. Based on BIOWIN v4.10, 3,5-dimethylhept-3-ene is predicted to be not readily biodegradable. It is a borderline case as the PBT screening criterion for Biowin 6 (probability <0.5) as stated in Table R.11-4 of the ECHA guidance (ECHA, 2014) is met, but the screening criteria for Biowin 2 (<0.5) and Biowin 3 3 (<2.25-2.75) are not met:

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 0.6874
Biowin2 (Non-Linear Model): 0.7714
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.9202 (weeks)
Biowin4 (Primary Survey Model): 3.6656 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): 0.3926
Biowin6 (MITI Non-Linear Model): 0.4370

Concerning **phototransformation in air**, 3,5-dimethylhept-3-ene has the potential to volatilize to air based on a high vapour pressure where it is subject to rapid atmospheric oxidation by means of hydroxyl radicals (OH·). Whether phototransformation in air will be effective for 3,5-dimethylhept-3-ene is dependent on the volatilization. However, branched alkenes are also hydrophobic and will bind to suspended particles and sediment, thus lowering the impact of volatilization.

To support the P assessment of 3,5-dimethylhept-3-ene, supporting data is used from the evalulations for C7- C9 isoalkanes (part of the OECD SIDS C7-C9 Aliphatic Hydrocarbon Solvents Category) and for EC 292-459-0, alkanes C9-12-iso (assessed by the TC NES subgroup on identification of PBT and vPvB Substances, PBT WORKING GROUP – PBT LIST No. 24) as well as from alkenes in the OECD SIDS Higher olefins category assessment report (2004) given the structural similarities with components of this substance.

C7-C9 isoalkanes (OECD, 2010)
Use of data for C7- C9 isoalkanes in the persistence assessment as was done for isoheptane in the substance evaluation report for EC No 250-610-8 is reasonable given the structural similarities, in particular with branched isoalkanes. The substances grouped in the C7-C9 isoalkanes subcategory are:

- CAS 142-82-5, Alkyl-branched C8 isoparaffin, 2,2,4-trimethylpentane
- CAS 70024-92-9 Alkanes, C7-8, iso- [a multi-constituent substance that can be composed predominantly of alkyl-branched C7 and C8 isoparaffin isomers that can include 2,2,4-trimethylpentane as a constituent; other constituents can include methyl- hexanes and heptanes, dimethyl- pentanes and hexanes, and trimethylpentanes]
- CAS 90622-56-3 Alkanes, C7-10, iso- [a multi-constituent substance that can be composed predominantly of branched C7, C8, and/or C9 isoparaffin isomers, which can include methyl- hexanes, heptanes, and/or octanes; dimethyl- pentanes, hexanes, and/or heptanes; and trimethylpentanes and/or –hexanes]

Biodegradation tests **in water** were performed with C7- C9 isoalkanes (CAS 90622-56-3) according to OECD Guideline 301 F or with methods equivalent to OECD Guideline 301F with activated sludge used for domestic wastewater treatment.

Degradation of test substance summarized from the two studies was the following: 10.5 - 26.83 % after 11-15 days, 51.3 % after 28 days, 49 - 60.3 % after 42 - 43 days, 60.2 % after 60 days, 61.81 - 64.06 % after 70 – 75 days (OECD, 2010).

The data show that C7 - C9 isoalkanes do not classify as readily biodegradable, but can demonstrate high extents of biodegradability when test durations are extended. However, interpreting the results of ready-tests for UVCBs is a complex issue that has been discussed for other substances suspected of PBT properties: it might be that some substances are degrading and others are not, causing incomplete mineralization.

EC 292-459-0, alkanes C9-12-iso
Use of data from the PBT evaluation for EC 292-459-0, alkanes C9-12-iso (ECB Summary Fact Sheet 24, 2008) in the persistence assessment is reasonable given the structural similarities with components of this substance. Selected 2- to 4-branched constituents of this UVCB-substance were concluded not to meet the P/vP criteria based on screening data. A biodegradation probability greater than 0.5 was considered as a screening criterion for "biodegrades fast". It was noted, that the bioHCwin–model significantly under-predicts the degradation half-lives of isoalkanes especially those having branches at the end(s) of the alkyl chain.

The calculated half-life of 3,5-dimethylhept-3-ene with BioHCwin is 3.307 days which is less than the estimated half-lives of 3.5 to 69 days for all typical constituents and realistic worst case constituents assessed for EC 292-459-0. These BioHCwin calculations considered only C11, C12 and cyclic components. Additional eMSCA calculations with BioHCwin for two C9 components result in half-lives of 7.6 and 11.0 days.

The PBT evaluation for EC 292-459-0 thus provides evidence to support that 3,5-dimethylhept-3-ene does not meet the P/vP criteria, since 3,5-dimethylhept-3-ene is estimated to be less persistent than components in EC 292-459-0 that were concluded not to meet the P/vP criteria.

OECD SIDS Higher olefins category assessment report (OECD, 2004)
Use of data from the OECD SIDS Higher olefins category in the persistence assessment is reasonable given the structural similarities, in particular with C7-C9 alkenes. A ready biodegradability test with 1-hexene demonstrated this substance to meet criteria to be considered readily biodegradable in an OECD 301C test, whereas considerable ultimate degradation was observed in a Modified Sturm test (22 % at 28 days). No ready biodegradability tests were reported for heptene, octane and nonene, but like for hexene all three substances are predicted to be readily biodegradable with BIOWIN. Branched C6-C9 alkenes are however expected to be more persistent compared to unbranched C6-C9 alkenes. Alkenes, C10-13 (linear) CAS 85535-87-1 showed 60-70% biodegradation after 28 days in two OECD 301D studies but it was not clear whether the 10 day window was met. Alkenes, C9-11, C10 Rich CAS 68526-56-7 showed 21% biodegradation by 28 days in an OECD 301F study.

Conclusion on Persistence Assessment

No experimental biodegradation data are available for 3,5-dimethylhept-3-ene. The substance is predicted to be not readily biodegradable and thus meets the P/vP screening criterion as a borderline case. Supporting data from alkenes and C6-C12 alkanes would suggest that 3,5-dimethylhept-3-ene has a potential to biodegrade. However, in the absence of experimental data on 3,5-dimethylhept-3-ene, the P assessment cannot be concluded. Since the substance does not fulfil the B/vB criteria, as discussed below, it is not necessary to investigate the biodegradation further in order to clarify the PBT concern.

Bioaccumulation assessment

QSAR estimated log Kow of 3,5-dimethylhept-3-ene is 4.53 (EPI Suite), just fulfilling the criterion of log Kow > 4.5 for screening a substance as potentially B. This Kow value results in an estimated log BCF of 2.655 (EPI suite, BCFBAFv3.02). The estimated BCF of 452.1 L/kg is evidence supporting that 3,5-dimethylhept-3-ene does not fulfil the B criterion BCF > 2000 L/kg.

Use of supporting data from 2,4,6-trimethyl-3-heptene (CAS 126690-66-2) as well as from the PBT evaluations for C7- C9 isoalkanes (OECD, 2010), EC 292-459-0, alkanes C9-12-iso (ECB Summary Fact Sheet 24, 2008) and EC 297-629-8 (ECB Summary Fact Sheet 62, 2008) is applied given the structural similarities with components of these substances.

Read-across to 2,4,6-trimethyl-3-heptene (CAS 126690-66-2)
QSAR models predict a significant higher bioaccumulation potential for 2,4,6-trimethyl-hept-3-ene compared to 3,5-dimethylhept-3-ene. For 2,4,6-trimethyl-hept-3-ene an experimental log BCF of 3.29 corresponding to a BCF of 1950 L/kg is reported by Dimitrov et al. (2005) although no experimental details are available. The fact that the experimental BCF for 2,4,6-trimethyl-hept-3-ene does not exceed the trigger of 2000 L/kg can be considered evidence to support that 3,5-dimethylhept-3-ene does not fulfil the B criterion.

C7-C9 isoalkanes (OECD, 2010)
Use of data from C7-C9 isoalkanes as was done for isoheptane in the substance evaluation report for EC No 250-610-8 is reasonable given the structural similarities of these hydrocarbons. In the category assessment of C7-C9 Aliphatic Hydrocarbon Solvents it was concluded that the C7-C9 isoalkanes (Iso-Paraffins Subcategory) have a low to moderate bioaccumulative potential:

"Category members are expected to sorb to organic matter in soil, sediment, and wastewater solids based on estimated log Koc values ranging from 3.0 to 4.7. Category members have a potential to bioaccumulate, based on a measured BCF value of 199 in a mussel (Mytilus edulis) for n-octane that used a limited study design and calculated BCF values (BCFBAF v3.0 model from the EPI Suite Program) that range from 105 (n-nonane) to 1216 (n-octane) (log BCF = 2.02 to 3.08) for the single substances. These predictions capture the range of log Kow within the category and do not consider biotransformation. These data suggest a low to moderate order of bioaccumulative potential for category members."

The OECD category assessment of C7-C9 Aliphatic Hydrocarbon Solvents also includes a study conducted in fathead minnow by Tolls and van Dijk (2002) with n-dodecane and 2,2,4,6,6-pentamethylheptane. The BCF value for n-dodecane was reported as <240 l/kg (n-dodecane was not detected in fish, therefore a BCF upper limit of 240 l/kg was calculated based on the median of aqueous concentrations during the experiment, 0.25 ug/L). In comparison, 2,2,4,6,6-pentamethylheptane was detected in fish and the BCF was reported as 880 l/kg (value was calculated based on the average fish/water concentration range measured during steady state). The BCFs of both compounds were small compared to the BCF predicted based on their hydrophobicity. The authors concluded that for both linear and branched hydrocarbons, it appears that efficient metabolism of the test compounds in fathead minnows prevents bioaccumulation. Thus the estimated BCF of 452.1 L/kg for 3,5-dimethylhept-3-ene which does not account for the known metabolism of hydrocarbons in fish is also likely to be an overestimation of the actual bioaccumulation potential in fish.

EC 292-459-0, alkanes C9-12-iso
Use of data from the PBT evaluation for EC 292-459-0 (ECB Summary Fact Sheet 24, 2008) in the bioaccumulation assessment is reasonable given the structural similarities with components of this substance. In the bioaccumulation assessment it was 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. Regarding the bioaccumulation potential of the parent no final conclusion was drawn.

EC 297-629-8, hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated

Use of data from the PBT evaluation for EC 297-629-8 (ECB Summary Fact Sheet 62, 2008) is justified owing to structural similarities with components of this substance. The bioaccumulation assessment concluded:

"Bioaccumulation: The substance does not meet the B criterion as a borderline case. An experimental BCF of 880 ± 438 L/kg was obtained for fish in a flow-through test for the main constituent 2,2,4,6,6-pentamethylheptane generally known, that the fish are able to metabolize effectively this kind of hydrocarbon substances. However, it is noted that no bioaccumulation data with other animals are available and they not be able to metabolize these substances as effectively as fish."

OECD SIDS Higher olefins category assessment report (OECD, 2004)

Use of data from the OECD SIDS Higher olefins category in the bioaccumulation assessment is reasonable given the structural similarities, in particular with C7-C9 alkenes. The QSAR estimated BCF for 3,5-dimethylhept-3-ene of 452 L/kg is between the QSAR estimated BCF of 236 L/kg for heptene and 659 L/kg for octene. The reliability of the QSAR estimates is difficult to judge in the absence of experimental BCF values for alkenes from the OECD SIDS Higher olefins category.

Conclusion on Bioaccumulation Assessment

No experimental bioaccumulation data are available for 3,5-dimethylhept-3-ene. The substance is predicted to have a Log Kow of 4.53 and thus meets the B/vB screening criterion. An estimated BCF of 452.1 L/kg (EPI suite, BCFBAFv3.02), indicates that 3,5-dimethylhept-3-ene does not fulfil the B criterion BCF > 2000 L/kg.

A measured BCF of 1950 is reported for the structurally-related alkene 2,4,6-trimethyl-hept-3-ene (Dimitrov et al, 2005) which is predicted to have similar physico-chemical properties to 3,5-dimethylhept-3-ene. This value is below the B criterion of 2000. However, experimental details of the BCF test are not available.

Measured fish BCFs are available for n-dodecane: <240 l/kg, and 2,2,4,6,6-pentamethylheptane: 880 l/kg. Both values are below the B criterion.

3,5-dimethylhept-3-ene is expected to be metabolised by fish as it is a hydrocarbon.

Overall, it can be concluded that 3,5-dimethylhept-3-ene does not meet the B/vB criterion because the fish BCF is predicted to be <2000 and measured data for alkenes/alkanes with similar structure and physicochemical properties support this conclusion.

Toxicity assessment

No experimental toxicity data were found for 3,5-dimethylhept-3-ene. Public MSDS data for hexene report an LC_{50} of 5.6 mg/L based on a OECD 203 test with rainbow trout (*Onchorhynchus mykiss*) (OECD, 2004). Acute toxicity studies with fish, Daphnia and algae for the whole test substance showed poor correlation between nominal and measured concentrations attributed to high volatility. Due to the high volatility of 3,5-dimethylhept-3-ene (estimated Henry Law Constant 1.18E+5 Pa m^3 mole-1) reliable testing of its effects on aquatic organisms is also anticipated to be difficult. In particular, algal tests with very volatile substances are technically very difficult to perform satisfactorily and may as a consequence yield results that are difficult to interpret and of limited relevance to real-world conditions (OECD, 2000). Adequate exposure would at least need to be validated by analytical measurements.

The following QSAR predictions were obtained for 3,5-dimethylhept-3-ene:

96-h LC_{50} for fish is 0.555 mg/L (ECOSAR v11).

48-h EC_{50} for daphnids is 0.396 mg/L (ECOSAR v11).

96-h EC50 for green algae is 0.447 mg/L (ECOSAR v11).

Use of data from the evaluations for C7- C9 isoalkanes (OECD, 2010), EC 292-459-0, alkanes C9-12-iso (ECB Summary Fact Sheet 24, 2008) and EC 297-629-8 (ECB Summary Fact Sheet 62, 2008) in the toxicity assessment is applied given the structural similarities with components of these substances.

C7-C9 isoalkanes (OECD, 2010)
Use of data from C7-C9 isoalkanes as was done for isoheptane in the substance evaluation report for EC No 250-610-8 is reasonable given structural similarities with components of this substance:

Acute toxicity

There are calculated and measured aquatic toxicity data for the single analogue chemical substance, 2,3,4-trimethylpentane (2,3,4-TMP) that are used as read-across data to 2,2,4-trimethylpentane (2,2,4-TMP), and measured acute aquatic toxicity data for hydrocarbons, C7-C9, isoalkanes (CAS No 90622-56-3).

Additionally, data from the multi-constituent subcategory can also be used as read-across data because these substances contain significant amounts of isoparaffins and have carbon number ranges that are similar to and overlap with the two multi-constituent members, CAS No 70024-92-9 and CAS No 90622-56-3. Calculated and measured 96-h fish LC_{50} values for two subcategory members range from 0.11 to 1.28 mg/L. Measured 48-hr daphnid data, 0.2 mg/L, and 96-h LC_{50} marine invertebrate data, 0.4 and 0.9 mg/L, are available for 2,3,4-TMP. These data are consistent with the data identified for the multi-constituent subcategory, which is expected given the reasons mentioned above. The alga data used to characterize the iso-paraffin subcategory are from the multi-constituent subcategory with a 72-h EC_{50} value of 0.4 mg/L.

Chronic toxicity

There are measured chronic aquatic toxicity data for one member of the multi-constituent subcategory, containing C7-C9 n-alkanes, isoalkanes, and cyclic alkanes. The 21-day LOEC value was 0.32 mg/L and the NOEC value was 0.17 mg/L, based on reproduction. The 21-day EC_{50} value from this study was 0.23 mg/L, based on survival. Additional estimated daphnid chronic toxicity data for n-heptane, 2,2,4-trimethylpentane, and nonane range from 0.23 to 0.06 mg/L.

EC 292-459-0, alkanes C9-12-iso
Use of data from the PBT evaluation for EC 292-459-0 (ECB Summary Fact Sheet 24, 2008) is reasonable given the structural similarities with components of this substance. The toxicology assessment concluded:

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.

EC 297-629-8, hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated
Use of data from the PBT evaluation for EC 297-629-8 (ECB Summary Fact Sheet 62, 2008) is applied given the structural similarities with components of this substance. The ecotoxicology assessment concluded:

Toxicity: The substance does not meet the T criterion as a borderline case. Experimental reliable long-term data are available for the main constituent 2,2,4,6,6-pentamethylheptane. Experimental reliable long-term data are available for Daphnia magna with a NOEC (21 days) of 0.013 mg/L from a semi-static OECD 211 test. Additionally, no effects were observed in a static algal inhibition test according to OECD 201 at a nominal (and initial measured) concentration of 0.40 mg/L ("worst case" NOEC (0-168 hours) > 0.0064 mg/L based on measured concentrations). According to ECOSAR v0.99h, fish ecotoxicity is not expected to differ significantly from the ecotoxicity to invertebrates and algae. Additionally, the substance is due to its structure not expected to elicit effects beyond the baseline toxicity.

OECD SIDS Higher olefins category assessment report

The OECD SIDS Higher Olefins-Category (OECD, 2004) reports a measured fish 96h LC_{50} of 5.6 mg/L for 1-hexene. This corresponds well with the ECOSAR estimated value of 6.16 mg/L which gives confidence in the ECOSAR predictions for alkenes. ECOSAR estimated fish LC_{50} values for heptene, octene and nonene are 2.09, 0.83 and 0.38 mg/l, respectively. The ECOSAR estimated Daphnia and green algae EC_{50} values for heptene, octane and nonene are similar. The ECOSAR estimated values for 3,5-dimethylhept-3-ene are in the same range.

Conclusion on (Eco)toxicity Assessment

No experimental aquatic ecotoxicity data are available for 3,5-dimethylhept-3-ene. The substance is predicted to have acute E/LC50 values between 0.4-0.6 mg/l. This is above the T screening criterion of E/LC50< 0.1mg/l.

The available mammalian toxicity data have not been assessed.

The available measured data for structurally related substances suggest a narrow range for aquatic acute toxicity of aliphatic hydrocarbons to fish, Daphnia and algae with L(E)C_{50} values around or below 1 mg/L. Overall, it seems not likely that 3,5-dimethylhept-3-ene fulfils criteria for T. However, no final conclusion can be drawn for the assessment of T.

OVERALL CONCLUSION

Overall, 3,5-dimethylhept-3-ene selected as representative worst case constituent for Reaction mass of 2-methylpent-2-ene and diisopropyl ether (EC No 906-484-8) is not considered a PBT substance. It does not meet the B criterion. No final conclusion can be drawn for the assessment of P and T.

7.12. Exposure assessment

Exposure assessment was not in the scope of eMSCA evaluation.

7.13. Risk characterisation

Risk characterisation was not in the scope of eMSCA evaluation.

7.14. References

Title	Author	Publication/source details	Date
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7.15. Abbreviations

BCF	Bioconcentration factor
CAS	Chemical Abstracts Service
CLP	Classification, Labelling and Packaging (of hazardous chemicals)
DNEL	Derived No Effect Level
ECHA	European Chemicals Agency
EPA	Environmental Protection Agency
EPIWIN	The EPI (Estimation Programs Interface) Suite™ is a Windows®-based suite of physical/chemical property and environmental fate estimation programs developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
OECD	Organization for Economic Cooperation and Development
QSAR	Quantitative Structure-Activity Relationship
PBT	Persistent Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SEv	Substance Evaluation
UVCB	Substances of Unknown or Variable composition, Complex reaction products or Biological materials.
vPvB	Very Persistent and Very Bioaccumulative