Justification Document for the Selection of a CoRAP Substance

Substance Name (Public Name):	Reaction mass of 2-methylpentane and Hexanol, branched and linear and diisopropyl ether
Chemical Group:	
EC Number:	906-390-7
CAS Number:	
Authority:	IT MSCA
Version:	22/03/2016

Note

This document has been prepared by the evaluating Member State given in the CoRAP update.

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1 IDENTITY OF THE SUBSTANCE

1.1 Other identifiers of the substance

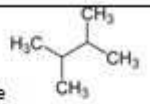
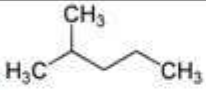
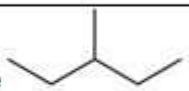
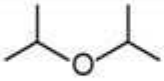
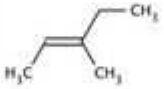
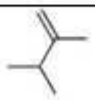
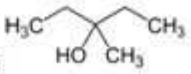
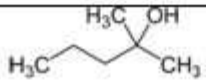
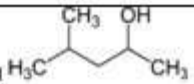
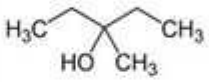
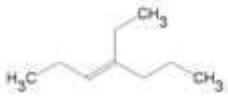
Table: Other Substance identifiers

EC name (public):	Reaction mass of 2-methylpentane and Hexanol, branched and linear and diisopropyl ether
IUPAC name (public):	
Index number in Annex VI of the CLP Regulation:	
Molecular formula:	A complex and variable combination of hydrocarbons having carbon numbers predominantly in the C3, C6 & C9 chain length and oxygenated organic molecules, predominantly diisopropyl ether and hexanol (branched and linear). See diagram
Molecular weight or molecular weight range:	ca. 96.0
Synonyms:	

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

Structural formula:

Main constituents of the Reaction Mass of 2-MethylPentane, Haxanol (branched and Linear) and Diisopropylether.

n-Propanol (NPA) 	2,3-dimethylbutane 
2-methylpentane 	3-methyl pentane 
Isopropyl Ether (IPE) 	3-methyl-2-pentene 
2,3 dimethylbutene 	3-methyl-2-pentanol 
2-methyl-2-pentanol 	4-methyl-2-pentanol 
2,4 dimethylheptane 	3,5 dimethyl-3-heptene 
Propyl isopropyl ether 	3-methyl-3-pentanol 
Propylene 	IPA 
4-ethyl-3-heptene 	

2 OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

Table: Completed or ongoing processes

RMOA	☐ Risk Management Option Analysis (RMOA)	
REACH Processes	Evaluation	☐ Compliance check, Final decision
		☐ Testing proposal
		☐ CoRAP and Substance Evaluation
	Authorisation	☐ Candidate List
		☐ Annex XIV
	Restri -ction	☐ Annex XVII[1]
Harmonised C&L	☐ Annex VI (CLP) (see section 3.1)	
Processes under other EU legislation	☐ Plant Protection Products Regulation Regulation (EC) No 1107/2009	
	☐ Biocidal Product Regulation Regulation (EU) 528/2012 and amendments	
Previous legislation	☐ Dangerous substances Directive Directive 67/548/EEC (NONS)	
	☐ Existing Substances Regulation Regulation 793/93/EEC (RAR/RRS)	
(UNEP) Stockholm convention (POPs Protocol)	☐ Assessment	
	☐ In relevant Annex	

[1] Entry no 59.

Other processes / EU legislation	☐ Other (provide further details below)

Other processes/EU legislation: Substance is included to the Annex III: LIST OF SUBSTANCES WHICH COSMETIC PRODUCTS MUST NOT CONTAIN EXCEPT SUBJECT TO THE RESTRICTIONS LAID DOWN (reference no 7) of the Regulation (EC) No 1223/2009 of the European Parliament and of the Council of 30 November 2009 on cosmetic products.

3 HAZARD INFORMATION (INCLUDING CLASSIFICATION)

3.1 Classification

3.1.1 Harmonised Classification in Annex VI of the CLP

Table: Harmonised classification

No harminised classification

3.1.2 Self classification

GHS

Aquatic Chronic 3;

Asp. Tox. 1; Flam. Liquid 2; STOT Single Exp. 3

3.1.3 Proposal for Harmonised Classification in Annex VI of the CLP

none

4 INFORMATION ON (AGGREGATED) TONNAGE AND USES[2]

4.1 Tonnage and registration status

Table: Tonnage and registration status

From ECHA dissemination site		
☒ Full registration(s) (Art. 10)	☐ Intermediate registration(s) (Art. 17 and/or 18)	
Tonnage band (as per dissemination site)		
☐ 1 – 10 tpa	☐ 10 – 100 tpa	☐ 100 – 1000 tpa
☒ 1000 – 10,000 tpa	☐ 10,000 – 100,000 tpa	☐ 100,000 – 1,000,000 tpa
☐ 1,000,000 – 10,000,000 tpa	☐ 10,000,000 – 100,000,000 tpa	☐ > 100,000,000 tpa
☐ <1 . . . . . >+ tpa (e.g. 10+ ; 100+ ; 10,000+ tpa)		☒ Confidential

4.2 Overview of uses

Table: Uses

Part 1:

☒ Manufacture	☒ Formulation	☒ Industrial use	☒ Professional use	☒ Consumer use	☐ Article service life	☐ Closed system

[2] *The ECHA dissemination site was accessed 19.05.2015.*

5. JUSTIFICATION FOR THE SELECTION OF THE CANDIDATE CoRAP SUBSTANCE

5.1. Legal basis for the proposal

☒ Article 44(2) (refined prioritisation criteria for substance evaluation)

☐ Article 45(5) (Member State priority)

5.2. Selection criteria met (why the substance qualifies for being in CoRAP)

☒ Fulfils criteria as CMR/ Suspected CMR

☐ Fulfils criteria as Sensitiser/ Suspected sensitiser

☐ Fulfils criteria as potential endocrine disrupter

☐ Fulfils criteria as PBT/vPvB / Suspected PBT/vPvB

☒ Fulfils criteria high (aggregated) tonnage (*tpa > 1000*)

☒ Fulfils exposure criteria

☐ Fulfils MS's (national) priorities

5.3 Initial grounds for concern to be clarified under Substance Evaluation

Hazard based concerns		
CMR ☐ C ☐ M ☐ R	Suspected CMR[3] ☐ C ☐ M ☐ R	☐ Potential endocrine disruptor
☐ Sensitiser	☐ Suspected Sensitiser[3]	
☐ PBT/vPvB	☒ Suspected PBT/vPvB[3]	☐ Other (please specify below)
Exposure/risk based concerns		
☒ Wide dispersive use	☐ Consumer use	☐ Exposure of sensitive populations
☐ Exposure of environment	☐ Exposure of workers	☐ Cumulative exposure
☒ High RCR	☐ High (aggregated) tonnage	☐ Other (please specify below)

[3] CMR/Sensitiser: known carcinogenic and/or mutagenic and/or reprotoxic properties/known sensitising properties (according to CLP harmonized or registrant self-classification or CLP Inventory)
Suspected CMR/Suspected sensitiser: suspected carcinogenic and/or mutagenic and/or reprotoxic properties/suspected sensitising properties (not classified according to CLP harmonized or registrant self-classification)
Suspected PBT: Potentially Persistent, Bioaccumulative and Toxic

- **Persistence**: At pH4, 7 and 9 there was less than 10% hydrolysis after 120 hours at 50°C when monitoring the isopropyl ether content of the test material, equivalent to a half-life greater than 1 year at 25°C. In a ready biodegradability test conducted according to guideline OECD 310, 22% biodegradation was observed in 28 days. The degradation simulation studies required at this tonnage band have been waived so no definite conclusion on P can be made. The screening criterion for P/vP is met.
- **Bioaccumulation**: The measured water solubility of the substance was found to be dependent on loading and ranged from 0.444-16.9 g/l at nominal loadings between 1 and 100g/l respectively. Log Pow was measured using the HPLC method EU Method A.8 giving values between 0.324 to 4.63. From the chromatographic profile, one component, peak 9, meets the screening criterion for B. The fish bioaccumulation study required at this tonnage band is waived. A summary of QSAR predictions is provided which concludes that 'highest BCF calculated was 173.9 L/kg, which was associated with the C6 aliphatic constituents'. Based on the measured Pow, some components of the substance are potentially bioaccumulative and this cannot be ruled out without further information, such as further justification of the QSAR predictions or further bioaccumulation testing.
- **Toxicity**: There is insufficient data to determine whether the T criterion is met. Reproductive toxicity and repeated dose toxicity studies are waived.. Acute toxicity studies with fish and Daphnia show LC50s in the 10-100 mg/l range based on nominal concentrations. For algae, the 72h ErC50 was 80mg/l (nominal concentration). However, these aquatic toxicity studies all used the WAF approach so the actual toxicity of individual components is unclear. Long-term aquatic toxicity studies are waived.
- **Exposure and risks**: There is wide dispersive use of the substance as a fuel sources, including consumer exposure. Potential risks to consumer are identified.

5.4 Preliminary indication of information that may need to be requested t clarify the concern

☒ Information on toxicological properties	☒ Information on physico-chemical properties
☒ Information on fate and behaviour	☒ Information on exposure
☒ Information on ecotoxicological properties	☐ Information on uses
☐ Information ED potential	☐ Other (provide further details below)

- Further tests to investigate the persistence and bioaccumulation of certain components of the substance. It is difficult to request such information for components of a substance under compliance check.
- Substance identity check to determine whether hexane is present
- Further tests to investigate long-term toxicity and ecotoxicity, if necessary.
- Information on exposure to clarify the risk to consumers

5.5 Potential follow-up and link to risk management

☐ Harmonised C&L	☒ Restriction	☒ Authorisation	☐ Other (provide further details)
Dependent on whether the definitive PBT criteria are met and whether risks to consumers are found.			