# Justification Document for the Selection of a CoRAP Substance

# – Update –

| | |
|---|---|
| **Substance Name (public name):** | Reaction mass of 2-methylpentane and Hexanol, branched and linear and diisopropyl ether |
| **EC Number:** | 906-390-7 |
| **CAS Number:** | NS |
| **Authority:** | Italy |
| **Date:** | 22/03/2016<br>20/03/2018 (1. Update) |

**Cover Note**

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

Table of Contents

1 IDENTITY OF THE SUBSTANCE 3

1.1 Other identifiers of the substance 3

2 OVERVIEW OF OTHER PROCESSES / EU LEGISLATION 5

3 HAZARD INFORMATION (INCLUDING CLASSIFICATION) 6

3.1 Classification 6
3.1.1 Harmonised Classification in Annex VI of the CLP 6
3.1.2 Self classification 6
3.1.3 Proposal for Harmonised Classification in Annex VI of the CLP 6

4 INFORMATION ON (AGGREGATED) TONNAGE AND USES 7

4.1 Tonnage and registration status 7

4.2 Overview of uses 7

5. JUSTIFICATION FOR THE SELECTION OF THE CANDIDATE CORAP SUBSTANCE 8

5.1. Legal basis for the proposal 8

5.2. Selection criteria met (why the substance qualifies for being in CoRAP) 8

5.3 Initial grounds for concern to be clarified under Substance Evaluation 8

5.4 Preliminary indication of information that may need to be requested to clarify the concern 9

5.5 Potential follow-up and link to risk management 9

# 1 IDENTITY OF THE SUBSTANCE

## 1.1 Other identifiers of the substance

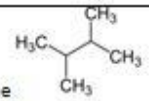
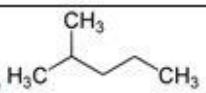
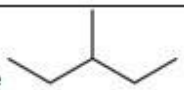
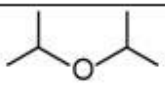
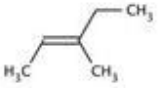
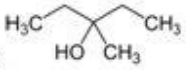
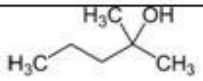
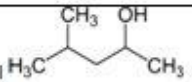
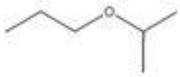
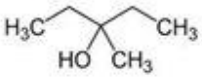
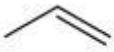
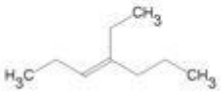
**Table: Other Substance identifiers**

| | |
|---|---|
| **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  | |

## 1.2 Similar substances/grouping possibilities

**Has read-across been used by the registrant for the concern related endpoints?** ☐ Yes ☒ No

**Is the substance a member of a category?** ☐ Yes ☒ No

# 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, Final decison |
| | | ☐ 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 | |
| Previ ous legisl ation | ☐ Dangerous substances Directive Directive 67/548/EEC (NONS) | |

[1] Please specify the relevant entry.

| | |
|---|---|
| | ☐ Existing Substances Regulation<br>Regulation 793/93/EEC (RAR/RRS) |
| (UNEP) Stockholm convention (POPs Protocol) | ☐ Assessment |
| | ☐ In relevant Annex |
| Other processes / EU legislation | ☐ Other (provide further details below) |
| *Please provide further details and more particularly specify where relevant if the process is ongoing or completed. Give only publicly available information.* | |

# 3 HAZARD INFORMATION (INCLUDING CLASSIFICATION)

## 3.1 Classification

### 3.1.1 Harmonised Classification in Annex VI of the CLP

The substance hasn't a harmonised classification

### 3.1.2 Self classification

- In the registration:
  - Asp. Tox. 1 H304
  - Flam. Liq. 2 H225
  - Aquatic Chronic 3 H412
  - STOT SE 3 H336

- The following hazard classes are in addition notified among the aggregated self classifications in the C&L Inventory:

  none

### 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 |
| This substance has 1 active registrations under REACH, 0 Joint Submission(s) and 1 Individual Submission(s). | | |

## 4.2 Overview of uses

This substance is used as a fuel by consumers, by professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing.

**Table: Uses**

**Part 1:**

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

**Part 3: There is high potential for exposure of**

| | |
|---|---|
| ☒ Humans | ☒ Environment |

[2] *The dissemination site was accessed in July 2017.*

# 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<br>☐ C ☐ M ☐ R | Suspected CMR[1]<br>☐ C ☐ M ☐ R | ☐ Potential endocrine disruptor |
| ☐ Sensitiser | ☐ Suspected Sensitiser[3] | |
| ☐ PBT/vPvB | ☒ Suspected PBT/vPvB[1] | ☐ 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 to 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 on 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.