

## Justification for the selection of a substance for CoRAP inclusion

|                                      |   |
|--------------------------------------|---|
| <b>Substance Name (Public Name):</b> | reaction mass of 2-methylpent-2-ene and diisopropyl ether |
| <b>Chemical Group:</b>               |   |
| <b>EC Number:</b>                    | 906-484-8   |
| <b>CAS Number:</b>                   | Not applicable  |
| <b>Submitted by:</b>                 | Slovenia  |
| <b>Published:</b>                    | 26/03/2014  |

### 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

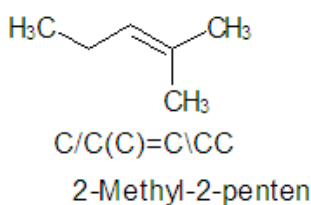
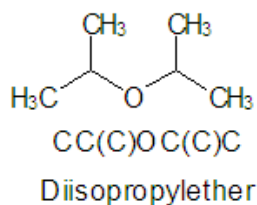
**Table 1: Substance identity**

|   |  |
|---|--|
| <b>EC name:</b>                                       | Reaction mass of 2-methylpent-2-ene and diisopropyl ether          |
| <b>IUPAC name:</b>                                    | Not applicable as multiconstituent substance.                      |
| <b>Index number in Annex VI of the CLP Regulation</b> | -  |
| <b>Molecular formula:</b>                             | Not applicable as multiconstituent substance                       |
| <b>Molecular weight or molecular weight range:</b>    | Not applicable as multiconstituent substance.                      |
| <b>Synonyms/Trade names:</b>                          | OC4 Produktstrom 7<br>reaction mass of DIPE and 2-methylpent-2-ene |

**Type of substance**     Mono-constituent     Multi-constituent     UVCB

#### Structural formula:

Main constituents



### 1.2 Similar substances/grouping possibilities

## 2 CLASSIFICATION AND LABELLING

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

Substance is not listed in Annex VI of CLP Regulation.

### 2.2 Self classification

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.

### 2.3 Proposal for Harmonised Classification in Annex VI of the CLP

None.

## 3 INFORMATION ON AGGREGATED TONNAGE AND USES

|  |   |  |   |
|--|---|--|---|
| From ECHA dissemination site   |   |  |   |
| <input type="checkbox"/> 1 - 10 tpa  | <input type="checkbox"/> 10 - 100 tpa                 | <input type="checkbox"/> 100 - 1000 tpa          |   |
| <input checked="" type="checkbox"/> 1000 - 10,000 tpa                        | <input type="checkbox"/> 10,000 - 100,000 tpa         | <input type="checkbox"/> 100,000 - 1,000,000 tpa |   |
| <input type="checkbox"/> 1,000,000 - 10,000,000 tpa                          | <input type="checkbox"/> 10,000,000 - 100,000,000 tpa | <input type="checkbox"/> > 100,000,000 tpa       |   |
| <input type="checkbox"/> <1 . . . . . >+ tpa (e.g. 10+ ; 100+ ; 10,000+ tpa) |   | <input type="checkbox"/> Confidential            |   |
|  |   |  |   |
| <input checked="" type="checkbox"/> Industrial use                           | <input checked="" type="checkbox"/> Professional use  | <input checked="" type="checkbox"/> Consumer use | <input checked="" type="checkbox"/> Closed System |
| Fuel, Fuel additives   |   |  |   |

## 4 JUSTIFICATION FOR THE SELECTION OF THE CANDIDATE CoRAP SUBSTANCE

### 4.1 Legal basis for the proposal

- Article 44(2) (refined prioritisation criteria for substance evaluation)
- Article 45(5) (Member State priority)

### 4.2 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

### 4.3 Initial grounds for concern to be clarified under Substance Evaluation

| Hazard based concerns   |  |  |
|---|--|--|
| CMR<br><input type="checkbox"/> C <input type="checkbox"/> M <input type="checkbox"/> R | Suspected CMR <sup>1</sup><br><input type="checkbox"/> C <input type="checkbox"/> M <input type="checkbox"/> R | <input type="checkbox"/> Potential endocrine disruptor     |
| <input type="checkbox"/> Sensitiser   | Suspected Sensitiser <sup>1</sup>  |  |
| <input type="checkbox"/> PBT/vPvB   | <input checked="" type="checkbox"/> Suspected PBT/vPvB <sup>1</sup>  | <input type="checkbox"/> Other (please specify below)      |
| Exposure/risk based concerns  |  |  |
| <input checked="" type="checkbox"/> Wide dispersive use                                 | <input type="checkbox"/> Consumer use  | <input type="checkbox"/> Exposure of sensitive populations |
| <input checked="" type="checkbox"/> Exposure of environment                             | <input type="checkbox"/> Exposure of workers   | <input type="checkbox"/> Cumulative exposure               |
| <input type="checkbox"/> High RCR   | <input checked="" type="checkbox"/> High (aggregated) tonnage  | <input type="checkbox"/> Other (please specify below)      |

<sup>1</sup> 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

The substance (reaction mass) contains diisopropyl ether and 2-methylpent-2-ene and various impurities with up to < 10 % in concentration. One impurity A\* (< 1 %) is suspected to have PBT properties. Water solubility = 2.8 g/L.

\* Besides the main constituents DIPE and 2-methylpent-2-ene, different impurities present in the reaction mass with typical concentrations of 0.8 – 6.4% are known. Some other impurities present at concentrations < 1% were identified through GC-MS analysis but could not be quantified. One C9-compound will be used as a representative structure for these low concentration impurities for the PBT/vPvB assessment. This C9-compound was chosen as a worst case example for bioaccumulation assessment.

#### B

Measured Log Kow using HPLC method ranged from 2.36 – 4.26 for main constituents and most impurities

Bioaccumulation studies waived.

Log Kow of impurity A =4.53 (QSAR, EPI Suite), BCF was estimated to 900 L/kg. Reg. concluded that this impurity is "*probably not B or vB*"

#### P

Screening test with reg. substance resulted in 20% degradation in 28d.

Simulation tests waived, Hydrolysis waived.

"In absence of further testing on the degradation of reaction mass of DIPE and 2-methylpent-2-ene in the environment, a potential for persistence of some of the constituents of this substance could in a first evaluation not be completely excluded as the substance is not readily degradable. The three components which are not predicted to be readily biodegradable (DIPE, 4-methylpent-1-ene and impurity A) are however volatile and are predicted to be removed by 99% from the atmosphere within 1 – 3 days. Based on these weights of evidence, all the components of reaction mass of DIPE and 2-methylpent-2-ene very probably do not fulfill the criteria for P nor for vP and are thus considered as *probably not P and not vP.*"

#### T

Short-term fish LC50=10 mg/L, long-term waived

Short-term daphnia 48h-EC50=6.9 mg/L, long-term waived

Micro-algae 72h-EC50=22 mg/L (based on growth rate)

Microorganism 3h NOEC=10 mg/L, 3h-EC20=330 mg/L, 3h-EC50=3000 mg/L.

Sediment and terrestrial toxicity waived

QSAR calculations for impurities do not meet the screening criteria for T. Only impurity A with an EC50 in the range 0.1 – 1 mg/L, was considered as possibly T.

To finally conclude on HH data results from 90d, PNDD and 2-Gen studies (3TPs) are needed.

#### 4.4 Other completed/ongoing regulatory processes that may affect suitability for substance evaluation

|   |   |
|---|---|
| <input type="checkbox"/> Compliance check, Final decision   | <input type="checkbox"/> Dangerous substances Directive 67/548/EEC  |
| <input checked="" type="checkbox"/> Testing proposal  | <input type="checkbox"/> Existing Substances Regulation 793/93/EEC  |
| <input type="checkbox"/> Annex VI (CLP)   | <input type="checkbox"/> Plant Protection Products Regulation 91/414/EEC  |
| <input type="checkbox"/> Annex XV (SVHC)  | <input type="checkbox"/> Biocidal Products Directive 98/8/EEC ;<br>Biocidal Product Regulation (Regulation (EU) 528/2012) |
| <input type="checkbox"/> Annex XIV (Authorisation)  | <input type="checkbox"/> Other (provide further details below)  |
| <input type="checkbox"/> Annex XVII (Restriction)   |   |
| <p><u>3 TPs:</u></p> <p>Sub-chronic toxicity (90 day): inhalation<br/>                 Reproductive toxicity (pre-natal developmental toxicity)<br/>                 Reproductive toxicity (two-generation reproductive toxicity)</p> <p>As there was not an unanimous agreement in MSC-30 about the third test, the case is referred to COM to prepare a decision in accordance with the procedure of Article 133(3) of REACH.</p> |   |

#### 4.5 Preliminary indication of information that may need to be requested to clarify the concern

|   |   |
|---|---|
| <input type="checkbox"/> Information on toxicological properties  | <input type="checkbox"/> Information on physico-chemical properties |
| <input checked="" type="checkbox"/> Information on fate and behaviour   | <input type="checkbox"/> Information on exposure                    |
| <input checked="" type="checkbox"/> Information on ecotoxicological properties  | <input type="checkbox"/> Information on uses                        |
| <input type="checkbox"/> Information ED potential   | <input type="checkbox"/> Other (provide further details below)      |
| <p>Based on the current data PBT properties cannot be excluded for the impurity A.</p> <p>The PBT concern is best addressed under Substance Evaluation since there is the possibility to request tests on impurities, which are suspected to have PBT properties.</p> |   |

#### 4.6 Potential follow-up and link to risk management

|   |                                      |  |  |
|---|--------------------------------------|--|--|
| <input type="checkbox"/> Harmonised C&L | <input type="checkbox"/> Restriction | <input type="checkbox"/> Authorisation | <input type="checkbox"/> Other (provide further details) |
|   |                                      |  |  |