Justification for the selection of a substance for CoRAP inclusion

Substance Name (Public Name):	Reaction mass of (1S,1'R)-2-[1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy]-2-methylpropyl propanoate, (1R,1'R)-2-[1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy]-2-methylpropyl propanoate and 2-methyl-2-{[(1R*,2R*)-2,6,6-trimethylcycloheptyl]oxy}propyl propanoate
Chemical Group:	
EC Number:	604-250-7
CAS Number:	141773-73-1
Submitted by:	Germany
Date:	17/03/2015

Note

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

Contents

1 IDENTITY OF THE SUBSTANCE

1.1 Other identifiers of the substance

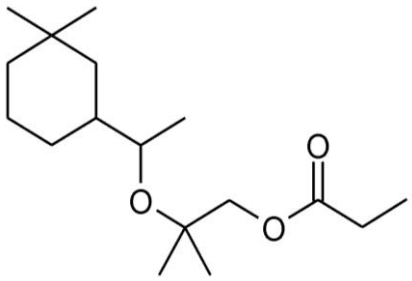
Table 1: Substance identity

EC name:	reaction mass of (1S,1'R)-2-[1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy]-2-methylpropyl propanoate, (1R,1'R)-2-[1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy]-2-methylpropyl propanoate and 2-methyl-2-{[(1R*,2R*)-2,6,6-trimethylcycloheptyl]oxy}propyl propanoate
IUPAC name:	reaction mass of (1S,1'R)-2-[1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy]-2-methylpropyl propanoate, (1R,1'R)-2-[1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy]-2-methylpropyl propanoate and 2-methyl-2-{[(1R*,2R*)-2,6,6-trimethylcycloheptyl]oxy}propyl propanoate
Index number in Annex VI of the CLP Regulation	N/A
Molecular formula:	$C_{17}H_{32}O_3$
Molecular weight or molecular weight range:	284.4 g·mol^{-1}
Synonyms/Trade names:	Helvetolide

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

Structural formula:

Disregarding stereochemistry, the first and the second component of the reaction mass can be represented as follows:



1.2 Similar substances/grouping possibilities

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2 CLASSIFICATION AND LABELLING

2.1 Harmonised Classification in Annex VI of the CLP

For the related substance "2-(1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy)-2-methyl propyl propanoate" with the same CAS number and the EC number 415-490-5, the following harmonised classification is included in Annex VI of the CLP regulation:

Table 2: Harmonised classification

Index No	International Chemical Identification	EC No	CAS No	Classification		Spec. Conc. Limits, M-factors	Notes
				Hazard Class and Category Code(s)	Hazard statement code(s)		
607-492-00-1	2-(1-(3',3'-dimethyl-1'-cyclohexyl) ethoxy)-2-methyl propyl propanoate	415-490-5	141773-73-1	Aquatic Chronic 2	H411		

2.2 Self classification

- In the registration:

  None in addition to the harmonized classification.

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

  Aquatic Chronic 1 H410

  Skin Irrit. 2 H315

2.3 Proposal for Harmonised Classification in Annex VI of the CLP

There is currently no proposal for harmonised classification registered or under consideration for this substance.

3 INFORMATION ON AGGREGATED TONNAGE AND USES

From ECHA 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

☐ Industrial use	☒ Professional use	☒ Consumer use	☐ Closed System

The substance is used in washing and cleaning products, polishes and wax blends as well as air care products and cosmetics.

4 OTHER COMPLETED/ONGOING REGULATORY PROCESSES THAT MAY AFFECT SUITABILITY FOR SUBSTANCE EVALUATION

☐ Compliance check, Final decision	☐ Dangerous substances Directive 67/548/EEC
☐ Testing proposal	☐ Existing Substances Regulation 793/93/EEC
☐ Annex VI (CLP)	☐ Plant Protection Products Regulation 91/414/EEC
☐ Annex XV (SVHC)	☐ Biocidal Products Directive 98/8/EEC ; Biocidal Product Regulation (Regulation (EU) 528/2012)
☐ Annex XIV (Authorisation)	☒ Other (provide further details below)
☐ Annex XVII (Restriction)	

For CAS No. 141773-73-1, a NONS registration with EC No. 415-490-5 exists.

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[1] ☐C ☐M ☐R	☐ Potential endocrine disruptor
☐ Sensitiser	☐ Suspected Sensitiser[1]	
☐ 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)

The substance fulfills the screening criteria for persistence and bioaccumulation as definded in Annex XIII, i.e.

P/vP criterion

The primary transformation product of Helvetolide, Helvetol, is not readily biodegradable. Therefore, the substance is considered to be potentially persistent.

B/vB criterion

The substance has a log Pow > 4.5. The available data on bioconcentration in fish require further evaluation. Helvetolide is therefore considered to be potentially bioaccumulative.
The primary transformation product Helvetol has a log P_{ow} of 4.33. Further information on bioaccumulation is required to clarify whether the transformation product is bioaccumulative or very bioaccumulative.

[1] 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

T criterion

The substance is self-classified as aquatic toxic 1 and 2. Long-term studies on aquatic ecotoxicology for daphnia are available for Helvetolide. No long-term studies on aquatic ecotoxicology for fish are available for Helvetolide. For a conclusion whether the T-criterion might be additionally fulfilled, information on toxicity on aquatic organisms might be also required. Under environmental conditions, Helvetolide degrades to Helvetol. No long-term studies on aquatic ecotoxicology are available for the transformation product. The toxic properties of Helvetol have to be assessed further.

The substance is used as fragrance in washing/cleaning products, polishes and wax blends, air care and cosmetic products. The use profile includes consumer and wide dispersive use. Therefore an environmental exposure is likely.

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 ED potential	☐ Other (provide further details below)
With regard to degradability and the bioaccumulation potential of the substance itself and the degradation product, further evaluation and, probably, further testing is required to clarify whether the substance needs to be considered as persistent, very persistent, bioaccumulative or very bioaccumulative. The long-term toxicity needs also to be assessed taking into account the effects of potential degradation products. Depending on the outcome of the P- and B-assessment, additional information on long-term aquatic ecotoxicity might also be required.	

5.5 Potential follow-up and link to risk management

☐ Harmonised C&L	☐ Restriction	☐ Authorisation	☐ Other (provide further details)
If the substance is identified as a PBT/vPvB substance, an analysis of risk management options will be provided, taking into account information on use and exposure. Potential options are the inclusion in the Candidate List, Authorisation or Restriction.			