Justification for the selection of a substance for CoRAP inclusion

Substance Name (Public Name):	A mixture of: 4-(2,2,3-trimethylcyclopent-3-en-1-yl)-1-methyl-2-oxabicyclo[2.2.2]octane; 1-(2,2,3-trimethylcyclopent-3-en-1-yl)-5-methyl-6-oxabicyclo[3.2.1]octane; spiro[cyclohex-3-en-1-yl-[(4,5,6,6a-tetrahydro-3,6',6',6'a-tetramethyl)-1,3'(3'aH)-[2H]cyclopenta[b]furan]; spiro[cyclohex-3-en-1-yl-[4,5,6,6a-tetrahydro-4,6',6',6'a-tetramethyl)-1,3'(3'aH)-[2H]cyclopenta[b]]furan]
Chemical Group:	Organic multi constituent substance
EC Number:	422-040-1
CAS Number:	426218-78-2
Submitted by:	SPAIN (Ministry of Agriculture, Food and Environment)
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:	A mixture of: 4-(2,2,3-trimethylcyclopent-3-en-1-yl)-1-methyl-2-oxabicyclo[2.2.2]octane; 1-(2,2,3-trimethylcyclopent-3-en-1-yl)-5-methyl-6-oxabicyclo[3.2.1]octane; spiro[cyclohex-3-en-1-yl-[(4,5,6,6a-tetrahydro-3,6',6',6'a-tetramethyl)-1,3'(3'aH)-[2H]cyclopenta[b]furan]; spiro[cyclohex-3-en-1-yl-[4,5,6,6a-tetrahydro-4,6',6',6'a-tetramethyl)-1,3'(3'aH)-[2H]cyclopenta[b]]furan]
IUPAC name:	Reaction mass of (1R)-5-methyl-1-[(1R)-2,2,3-trimethylcyclopent-3-en-1-yl]-6-oxabicyclo[3.2.1]octane and (1S)-3,6',6',6a'-tetramethyl-4',5',6',6a'-tetrahydro-3a'H-spiro[cyclohex-3-ene-1,3'-cyclopenta[b]furan] and (1S)-5-methyl-1-[(1R)-2,2,3-trimethylcyclopent-3-en-1-yl]-6-oxabicyclo[3.2.1]octane and 4-methyl-1-[(1R)-2,2,3-trimethylcyclopent-3-en-1-yl]-2-oxabicyclo[2.2.2]octane
Index number in Annex VI of the CLP Regulation	601-074-00-2
Molecular formula:	C16H26O
Molecular weight or molecular weight range:	234.37
Synonyms/Trade names:	*CASSIFFIX*

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

Structural formula:

1.2 Similar substances/grouping possibilities

There is no available information on other similar substances.

2 CLASSIFICATION AND LABELLING

2.1 Harmonised Classification in Annex VI of the CLP

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)		
601-074-00-2	See 1.1	422-040-1	-	Skin Irrit. 2 Eye Irrit. 2 Aquatic Chronic 2	H315 H319 H411	-	-

2.2 Self classification

- In the registration

R51/53 - Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment
R36/38 - Irritating to eyes and skin

Same hazards has been identified.

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

  Aquatic Chronic 4: H413

2.3 Proposal for Harmonised Classification in Annex VI of the CLP

None

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
In addition to the given tonnage band, there is a NONS registration for which the tonnage is confidential.		

☒ Industrial use	☒ Professional use	☒ Consumer use	☐ Closed System
The substance is an odour fragrance, with manufacture, industrial use and professional and consumer use. Focal and wide dispersive emissions.			

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)	
The substance was being assessed under the NONS procedure. This procedure has been closed since it was agreed that additional information for removing the concerns identified in this document could not be requested vía the Spanish initial NONS decision.	

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)

Persistence

Information regarding abiotic degradation refers to hydrolysis. The hydrolysis did not show a first order kinetic and therefore the DT50s were read from the graphs. The DT50 at pH 4, 7 and 9 were 710 hours (30 days), 520 hours (22 days) and 830 hours (35 days) at 25ºC. Regarding PBT properties, these data should be extrapolated to the default Tª of 12ºC which would increase the DT50s. No data on photo transformation is included.

A biodegradation test OECD 301D results in 3% biodegradation after 28 days. The substance was not found to be inhibitory to activated sludge bacteria. Therefore, the substance must be considered as not rapidly biodegradable.

According to the available information on degradation, CASSIFFIX is considered a P/vP substance.

[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

Bioaccumulation

No assays on bioaccumulation are included in the registration dossier. BCF values are estimated in eartworms as 121 l/kg ww and fish as 501 L/kg ww.

Taking into account the estimated log Pow of 4 used in the CSA, bioaccumulation potential is considered to be likely.

Toxicity

According to the toxicity information included in the registration dossier acute toxicity tests were provided for fish (96h-EC50 = 3.8 mg/L), aquatic invertebrates (48h-EC = 1.3 mg/L) and algae (72h-EC50 = 1.3 mg/L). Only chronic information is provided for algae (72h-NOEC = 2.6 mg/L).

Long-term information regarding aquatic invertebrates has not been provided. This information is relevant not only for the final the exposure assessment but also to remove uncertainties on PBT charateristics, since, according to the information provided, the substance is considered P and B.

Exposure

According to the information of the CSR analyzed, the substance is classified for the environment as R51/53 – H411, and therefore the exposure assessment and risk characterization has been performed, resulting all the Risk Characterization Ratios (RCRs) <1. Nevertheless, some concerns rise from the RCRssoil and the physico-chemical characteristics of this substance:

- Regarding the exposure scenario for Formulation it is confirmed the application of the STP sludge to agricultural soil,
- Environmental Release Categories (ERCs) also indicate wide dispersive uses (8d),
- According to Annex VIII, no soils toxicity information is provided and, when needed, the Equilibrium Partitioning Method (EPM) is applied for the stimations,
- In five of the exposure scenarios RCRs close to 1 have been calculated for agricultural soils (EPM approach),
- Potential increases of the tonnage, without additional notification, according the range of tonnage for the annex VIII (10-100 tons) would result in RCRs >1 for the soil compartment. This would indicate a potential risk and the need to investigate further the effects of the substance and/or degradation products on terrestrial organisms,
- The substance is stated as Persistent and not very high adsorptive but soil is identified as the compartment of concern,
- According to ECHA Guidance[2] R.7c (Table R.7.11-2), the substance falls under soil hazard category 3[3]. Although, it should also be highlighted that the LC50 of 1.3 mg/L (geometric mean of 1 -1.6 mg/L) for daphnia would confirm the concern on soil due to the proximity of the threshold to be considered as very toxic substance and the fulfilment of the criteria for the soil hazard category 4[4] .

According to the ECHA Guidance (R.7c Table R.7.11-2) the screening assessment based on EPM

[2] Guidance on information requirements and chemical safety assessment (November 2012).

[3] SHC3: The substance is persistent and not very toxic to aquatic organisms (EC/LC50 > 1 mg/L for algae, daphnia or fish).

[4] SHC4: Persistence and indication that the substance is very toxic to aquatic organisms (EC/LC50 ≤ 1 mg/L).

is not recommended to derive the PNEC soil as the intrinsic properties indicate a high hazard potential to soil organisms. Based upon the available aquatic toxicity information and the physico-chemical properties of the substance, and in relation to section R.7.11.6., Chapter R.7c of the ECHA guidance, the Spanish CA considers that the substance would fall into soil hazard category 3. The Guidance foresees in these cases that confirmatory long-term soil toxicity test should be conducted.

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)

In order to clarify potential T:

Long-term toxicity on aquatic invertebrates – Daphnia magna reproduction test (Annex IX, 9.1.5.); test method: EU C.20./OECD 211;

As the registrant confirms that soil application is expected, the substance falls under the soil category hazard 3 and the RCRs for soil compartment are very close to 1, even although the Annex VIII does not require information on soil compartment, due to the above rationale the registrant is requested to submit the following information regarding Classifix:

In order to get reliable information on effects on the soil compartment and remove uncertainties of RCR c.a 1:

1. Effects on terrestrial organisms – Effects on soil micro-organisms (Annex IX, 9.4.2.; test method: Soil microorganisms: nitrogen transformation test, EU C.21./OECD 216;

2. Effects on terrestrial organisms - Long-term toxicity to terrestrial invertebrates (Annex X, 9.4.4.); test method: Earthworm reproduction test (Eisenia fetida/Eisenia Andrei) OECD 222; or Enchytraeid reproduction test OECD 220; or Collembolan reproduction test in soil OECD 232.

5.5 Potential follow-up and link to risk management

☐ Harmonised C&L	☐ Restriction	☐ Authorisation	☒ Other (provide further details)

Potential follow-up will depend on the result of the evaluation.

CASSIFFIX is a NONS substance. Therefore, regarding this substance and regarding the NONS procedure, it was considered that the concerns identified in this document could not be solved since no additional information could be requested under the NONS decision. Therefore, additional long-term information could be requested under the CoRAP procedure to remove uncertainties regarding the soil compartment and PBT properties.