SUBSTANCE EVALUATION CONCLUSION

as required by REACH Article 48

and

EVALUATION REPORT

for

a mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol

(Florosa)

EC No 405-040-6

CAS No 63500-71-0

Evaluating Member State(s): Spain

Dated: May 2017

Evaluating Member State Competent Authority

Ministry of Agriculture, Food and Environment
Plaza de San juan de la Cruz s/n
28071 - Madrid
Spain
Tel: +34 91 597 5650
Fax:
Email: ogonzalez@mapama.es

Year of evaluation in CoRAP: 2012

Before concluding the substance evaluation a Decision requesting further information was issued on: 24 February 2014

Further information on registered substances here:

http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances

DISCLAIMER

This document has been prepared by the evaluating Member State as a part of the substance evaluation process under the REACH Regulation (EC) No 1907/2006. The information and views set out in this document are those of the author and do not necessarily reflect the position or opinion of the European Chemicals Agency or other Member States. The Agency does not guarantee the accuracy of the information included in the document. Neither the Agency nor the evaluating Member State nor any person acting on either of their behalves may be held liable for the use which may be made of the information contained therein. Statements made or information contained in the document are without prejudice to any further regulatory work that the Agency or Member States may initiate at a later stage.

Foreword

Substance evaluation is an evaluation process under REACH Regulation (EC) No. 1907/2006. Under this process the Member States perform the evaluation and ECHA secretariat coordinates the work. The Community rolling action plan (CoRAP) of substances subject to evaluation, is updated and published annually on the ECHA web site[1].

Substance evaluation is a concern driven process, which aims to clarify whether a substance constitutes a risk to human health or the environment. Member States evaluate assigned substances in the CoRAP with the objective to clarify the potential concern and, if necessary, to request further information from the registrant(s) concerning the substance. If the evaluating Member State concludes that no further information needs to be requested, the substance evaluation is completed. If additional information is required, this is sought by the evaluating Member State. The evaluating Member State then draws conclusions on how to use the existing and obtained information for the safe use of the substance.

This Conclusion document, as required by Article 48 of the REACH Regulation, provides the final outcome of the Substance Evaluation carried out by the evaluating Member State. The document consists of two parts i.e. A) the conclusion and B) the evaluation report. In the conclusion part A, the evaluating Member State considers how the information on the substance can be used for the purposes of regulatory risk management such as identification of substances of very high concern (SVHC), restriction and/or classification and labelling. In the evaluation report part B the document provides explanation how the evaluating Member State assessed and drew the conclusions from the information available.

With this Conclusion document the substance evaluation process is finished and the Commission, the Registrant(s) of the substance and the Competent Authorities of the other Member States are informed of the considerations of the evaluating Member State. In case the evaluating Member State proposes further regulatory risk management measures, this document shall not be considered initiating those other measures or processes. Further analyses may need to be performed which may change the proposed regulatory measures in this document. Since this document only reflects the views of the evaluating Member State, it does not preclude other Member States or the European Commission from initiating regulatory risk management measures which they deem appropriate.

[1] http://echa.europa.eu/regulations/reach/evaluation/substance-evaluation/community-rolling-action-plan

Contents

Part A. Conclusion

1. CONCERN(S) SUBJECT TO EVALUATION

A mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; transtetrahydro-2-isobutyl-4-methylpyran-4-ol (Florosa) was originally selected for substance evaluation in order to clarify concerns about:

- exposure,

- wide dispersive use and,

- high risk characterization ratio(s) for the environment.

During the evaluation no other concerns were identified.

Before concluding the substance evaluation the Decision requesting further information in order to clarify the initial concerns was issued on 24 February 2014.

2. OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

No other process or specific EU legislation has being identified regarding the risk assessment or the management of this substance.

3. CONCLUSION OF SUBSTANCE EVALUATION

The evaluation of the available information on the substance has led the evaluating Member State (eMSCA) to the following conclusion, as summarised in the table below.

Table 1. Conclusion on substance evaluation.

CONCLUSION OF SUBSTANCE EVALUATION Conclusions	Tick box
Need for follow-up regulatory action at EU level	
Harmonised Classification and Labelling	
Identification as SVHC (authorisation)	
Restrictions	
Other EU-wide measures	
No need for regulatory follow-up action at EU level	X

4. FOLLOW-UP AT EU LEVEL

4.1. Need for follow-up regulatory action at EU level

Not applicable.

4.1.1. Harmonised Classification and Labelling

4.1.2. Identification as a substance of very high concern, SVHC (first step towards authorisation)

4.1.3. Restriction

4.1.4. Other EU-wide regulatory risk management measures

5. CURRENTLY NO FOLLOW-UP FORESEEN AT EU LEVEL

5.1. No need for regulatory follow-up at EU level

Table 2. Reason for removed concern

REASON FOR REMOVED CONCERN The concern could be removed because	Tick box
Clarification of hazard properties/exposure	X
Actions by the registrants to ensure safety, as reflected in the registration dossiers (e.g. change in supported uses, applied risk management measures, etc.)	

The initial environmental assessment of the mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol (Florosa) was carried out using the information presented by the registrants and the default exposure values according to the CHESAR/EUSES models and specific emission rates by IFRA (2012). Due to the high production/formulation volume, the lack of information on both, real emissions and the existence of management measures, default emissions exposure values have been used for this environmental risk assessment, which concluded with the confirmation of an unacceptable risk for the environment, RCR >1, for the production, compounding and formulation life cycle stages for STPs, and the aquatic, sediment and soil compartments, at several sites.

Therefore, to confirm the environmentally safe use of the substance, the following information was requested in the Decision issued on 24/02/2014:

1. Short-term growth inhibition study aquatic plants (algae preferred) (Annex VII, 9.1.2; test method: Algae, Growth Inhibition Test, EU C.3/OECD201).

2. Information to refine the exposure assessment regarding:
- Operational Conditions (OC) (including specific environmental conditions);
- Risk Management Measures (RMM);
- Release rate measurements during the emission period of releases to environmental compartments.
  The above had to be provided for the production, compounding and formulation life cycle stages, as well as for two STPs and aquatic, soil and sediment environmental compartments at different sites.

The information requested in the Decision was provided by the registrants with the higher volume of production and use in August 2014 and in June 2015. The information provided by these registrants was enough to remove the identified concerns on exposure, wide dispersive use and high risk characterization ratio(s) for the environment. Therefore, no follow-up action at EU level is considered to be needed at this time.

5.2. Other actions

No further actions/risk management measures are considered to be needed at this time.

6. TENTATIVE PLAN FOR FOLLOW-UP ACTIONS (IF NECESSARY)

Not applicable.

Part B. Substance evaluation

7. EVALUATION REPORT

7.1. Overview of the substance evaluation performed

The mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol (Florosa) was originally selected for substance evaluation in order to clarify concerns about:

- exposure,

- wide dispersive use and,

- high risk characterization ratio(s) for the environment.

During the evaluation no other concerns were identified.

Table 3. Evaluated endpoints.

EVALUATED ENDPOINTS	
Endpoint evaluated	**Outcome/conclusion**
Environmental exposure	Information on exposure was required in order to enable the evaluating MSCA (eMSCA) to refine the exposure assessment and reduce the unacceptable risk characterization ratio for the environment identified as ground of concern. After the consideration of the exposure assessment carried out by the eMSCA it was concluded that there is no need for further actions or risk management measures.
Wide dispersive use	
High risk characterization ratio for the environment	

7.2. Procedure

The substance was initially not classified as hazardous for the environment, based on uncertain and incomplete information, and therefore, the environmental exposure assessment was not included in the registration dossier.

The initial assessment was targeted on the initial environmental concerns identified by the eMSCA: exposure, wide dispersive use and high RCR(s) for environmental compartments (aquatic, sediments and soil). These initial concerns were confirmed after the initial environmental assessment of the substance. This initial assessment was carried out using the information presented by the registrants and the default exposure values according to the CHESAR/EUSES models. During the evaluation the eMSCA did not identifiy any other concern.

Due to the high production/formulation volume, the lack of information on both, real emissions and the existence of risk management measures, EUSES default emissions values were used for the environmental risk assessment. IFRA emission rates (IFRA, 2012) were also applied as a second refinement. Both assessements concluded with the confirmation of an unacceptable risk for the environment, RCRs >1. These results were associated to the following stages: production, compounding and formulation, STPs, and the aquatic, sediment and soil compartments, at several plant-sites.

After the Decision was published and new specific exposure information was provided by the registants, the refinement of the initial assessment was carried out by the eMSCA.

The individual information provided by each of the 5 registrant companies in 5 different dossiers, has been compiled, analysed and considered for this assessment. Relevant higher tonnage declared by each company has been considered for the exposure estimations.

Most of the information provided by the registrants and needed for the assessment was generated in the 90's. No new information was generated by the registrants regarding the ecotoxicity endpoints, but the relevant endpoint conclusions were checked against those studies notified to the Spanish CA under a previous notification procedure of the substance in 2006.

7.3. Identity of the substance

The substance is a multi constituent substance having the following characteristics and physical–chemical properties (see also the IUCLID dataset for further details) (Table 5).

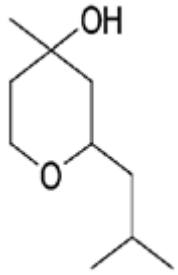
Table 4. Substance identity.

SUBSTANCE IDENTITY	
Public name:	A mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol
EC number:	405-040-6
CAS number:	63500-71-0
Index number in Annex VI of the CLP Regulation:	603-101-00-3
Molecular formula:	C_{10} H_{20} O_2
Molecular weight range:	172.268
Smiles notation:	CC(C)CC1CC(CCO1)(C)O
Synonyms:	Tetrahydro-2-isobutyl-4-methylpyran-4-ol, mixed isomers (*cis* and *trans);* CIS/TRANS-TIMO; Floral pyranol; Florol; Florosa; Florosol; Tetrahydro-4-methyl-2-(2-methylpropyl) -2H-pyran-4-ol; Pyranol;

	FLOROTYL; Keflorol; Reaction mass of (rel-2R,4R)-tetrahydro-4-methyl-2-(2-methylpropyl)-2H-pyran-4-ol and (rel-2R,4S)-tetrahydro-4-methyl-2-(2-methylpropyl)-2H-pyran-4-ol; Reaction mass of cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol and trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol; TETRAHYDRO-2-ISOBUTYL-4-METHYL-4(2H)-PYRANOL; Tetrahydro-4-methyl-2-(2-methylpropyl)-2H-pyran-4-ol

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

Structural formula:



Multiconstituent/UVCB substance/others

Name: a mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol has the following constituents:

Table 5. Constituents of the substance

Constituents
(rel-2R,4R)-tetrahydro-4-methyl-2-(2-methylpropyl)-2H-pyran-4-ol CAS: 65418-69-1
(rel-2R,4S)-tetrahydro-4-methyl-2-(2-methylpropyl)-2H-pyran-4-ol CAS: 65418-70-4

7.4. Physico-chemical properties

The mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol has the following characteristics and physical–chemical properties (Table 6).

Table 6. Overview of physico-chemical properties and values used for CSA.

OVERVIEW OF PHYSICOCHEMICAL PROPERTIES	
Property	**Values**
Physical state at 20°C and 101.3 kPa	*liquid*
Vapour pressure	*0.01 hPa at 20 ºC*
Water solubility	*23.653 mg/L at 23 ºC*
Partition coefficient n-octanol/water (Log Kow)	*1.65 at 23 ºC (measured)*
Flammability	*Non flammable liquid.*
Explosive properties	*Non explosive liquid.*
Oxidising properties	*Not oxidising.*
Granulometry	*Not applicable.*
Stability in organic solvents and identity of relevant degradation products	*Not applicable. The stability of the substance is not considered as critical.*
Dissociation constant	*Not applicable. The substance does not contain any ionic structure.*

7.5. Manufacture and uses

The information provided by each individual registrant has been analysed and summarised by the eMSCA in order to have a picture, as complete as possible, on those aspects that can be useful for the environmental risk assessment.

7.5.1. Quantities

The aggregated tonnage per year is included in the range 1,000 – 10,000 t/year.

Table 7. Tonnage range.

AGGREGATED TONNAGE (PER YEAR)				
☐ 1 – 10 t	☐ 10 – 100 t	☐ 100 – 1000 t	☒ **1000- 10,000 t**	☐ 10,000-50,000 t
☐ 50,000 – 100,000 t	☐ 100,000 – 500,000 t	☐ 500,000 – 1000,000 t	☐ > 1000,000 t	☐ Confidential

7.5.2. Overview of uses

The substance is a colourless organic liquid with a floral odour, used as an odour agent in fragrance blends and perfumes, consumer products, such as fine fragrance, personal/home care products, fabric care and laundry products. Therefore, not all identified uses of the evaluated substance take place in closed systems.

Identified uses published at the ECHA dissemination website in 2015 have been included in Table 8. All registrants have indicated the same uses. Only those use descriptors relevant for environmental emissions have been considered for this assessment. The information on use descriptors has been taken from the ECHA website and is in agreement with the information provided by registrants in their registration dossiers.

Table 8. Identified uses (published at the ECHA dissemination website, 2015).

USES	**Use(s)**
Formulation	**Industrial Compounding/formulation of Tetrahydro-4-methyl-2-(2-methylpropyl) -2H-pyran-4-ol** PROC 1: Use in closed process, no likelihood of exposure PROC 3: Use in closed batch process (synthesis or formulation) PROC 5: Mixing or blending in batch processes for formulation of preparations and articles (multistage and/or significant contact) PROC 8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities PROC 8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities PROC 9: Transfer of substance or preparation into small containers (dedicated filling line, including weighing) PROC 14: Production of preparations or articles by tabletting, compression, extrusion, pelletisation PROC 15: Use as laboratory reagent ERC 2: Formulation of preparations
Uses at industrial sites	**Use in Cleaning agents – at industrial sites** PROC 1: Use in closed process, no likelihood of exposure PROC 2: Use in closed, continuous process with occasional controlled exposure PROC 4: Use in batch and other process (synthesis) where opportunity for exposure arises PROC 7: Industrial spraying PROC 8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities PROC 10: Roller application or brushing PROC 13: Treatment of articles by dipping and pouring ERC 4: Industrial use of processing aids in processes and products, not becoming part of articles
Uses by professional workers	**Use in cleaning agents - professional** PROC 1: Use in closed process, no likelihood of exposure

	PROC 2: Use in closed, continuous process with occasional controlled exposure PROC 4: Use in batch and other process (synthesis) where opportunity for exposure arises PROC 8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities PROC 8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities PROC 10: Roller application or brushing PROC 11: Non industrial spraying PROC 13: Treatment of articles by dipping and pouring ERC 8a: Wide dispersive indoor use of processing aids in open systems ERC 8d: Wide dispersive outdoor use of processing aids in open systems
Consumer Uses	**Use of Cleaning Agents – Consumer** PC 8: Biocidal products (e.g. disinfectants, pest control) PC 28: Perfumes, fragrances PC 31: Polishes and wax blends PC 35: Washing and cleaning products (including solvent based products) PC 39: Cosmetics, personal care products ERC 8a: Wide dispersive indoor use of processing aids in open systems ERC 8d: Wide dispersive outdoor use of processing aids in open systems
Article service life	no
Uses advised against	Regarding consumer uses (C-1: Products with potential for significant oral contact), Tetrahydro-4-methyl-2-(2-methylpropyl) -2H-pyran-4-ol is not an approved flavour and should not be used in products with potential for significant oral contact (e.g Toys).

7.6. Classification and Labelling

7.6.1. Harmonised Classification (Annex VI of CLP)

The classification of the substance is given according to the entry in table 3.1 in Annex VI of CLP Regulation (Regulation (EC) 1272/2008).

Table 9. Harmonised classification according to Annex VI of the CLP Regulation.

HARMONISED CLASSIFICATION ACCORDING TO ANNEX VI OF CLP REGULATION (REGULATION (EC) 1272/2008)							
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)**		
603-101-00-3	Tetrahydro-2-isobutyl-4-methylpyran-4-ol, Reaction mass aus Isomeren (cis und trans)	405-040-6	63500-71-0	Eye Irrit. 2	H319	-	-

Labelling:

Pictogram GHS07 (exclamation mark), Signal word “Warning”, Hazard statement H319 (causes serious eye irritation)

7.6.2. Self-classification

n.a.

7.7. Environmental fate properties

Only the relevant information on fate properties, agreed by the eMSCA and relevant for this assessment, has been compiled in this report.

7.7.1. Degradation

Abiotic degradation

No hydrolysis study is provided, but due to structural properties of the substance, hydrolysis is not expected, therefore, the substance is considered as not hydrolysable.

No study is provided regarding phototransformation in air, but some indication can be obtained by using the degradation rate constant of 0.00000000004649 cm^3/molecule-sec, which results in a expected half life of the substance in air of 8.28 h at 25ºC (SRC AOPWIN v1.92) (unnamed report, 2009 - referred at the ECHA dissemination website). Additionally, half-life of ca. 2 days has been estimated by using the EUSES 2.1 programme.

No phototransformation in water nor soil is expected considering a degradation rate of 0 estimated by the EUSES 2.1.

Biodegradation

The substance is considered as not ready biodegradable (0-10% degradation after 28 d, under activated sludge, non-adapted OECD Guideline 301 B) (unnamed report, 1992 - referred at the ECHA dissemination website), therefore, without any additional information, poorly biodegradation rates are expected in surface water.

No study is available regarding biodegradation in soil, but as the substance is poorly biodegradable in water comparable low biodegradation rates are expected in soil.

Thus, the substance is considered poorly biodegradable regarding aquatic, sediments and soil compartments.

7.7.2. Environmental distribution

Adsorption/desorption

A study on adsorption (soil/sewage sludge) HPLC estimation method OECD Guideline 121, results in a measured log Koc of ca. 1.4 (unnamed report, 2007 - referred at the ECHA dissemination website). According to this value, adsorption to solid soil phase is not expected.

Volatilisation

Information regarding volatilisation to air is provided based on a calculated Henry's Law constant H of 0.00171 Pa m³/mol at 25 °C (SRC HENRYWIN v3.10 -Bond estimation method) (unnamed, 2009 - referred at the ECHA dissemination website).

A Henry´s Law constant of 0.01 Pa m³/mol is additionally calculated. The calculated Henry's law constant indicates that evaporation of the substance from water into the atmosphere is not greatly expected. A low/moderate evaporation rate of the substance from the surface water into the atmosphere is expected.

Based on the information available the substance is not highly adsorptive that indicates that soil and sediment are not expected to be the main target compartments for exposure assessment.

7.7.3. Bioaccumulation

No experimental study on bioaccumulation is provided in the registration dossier. The mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol is not expected to bioaccumulate in aquatic organisms due to a low log Pow of 1.65 measured for the substance. This log Pow value results in a BCF of 5.7 by the EPIWIN model (BAFBCF 3.01).

According to the estimated BCF of 5.7, the mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol is considered as non bioaccumulative substance. Same conclusion can be derived for the terrestrial compartment based on the log Pow.

Secondary poisoning

Based on the Log Pow of 1.65, a significant accumulation in organisms is not expected. Additionally, the partially polar structure and low molecular weight (<400) would indicate that a long biological half-life of the substance in tissues is not expected.

Therefore, secondary poisoning is of no concern for this substance.

7.8. Environmental hazard assessment

Only the relevant information for hazard assessment, agreed by the eMSCA and relevant for this assessment, has been compiled in this report.

7.8.1. Aquatic compartment (including sediment)

The substance is not ready biodegradable and the ecotoxicological data on fish, Daphnia and algae resulted in an LC50 of 354 mg/L for Oncorhynchus mykiss, an EC50 of ca. 320 mg/L for D. magna, and an EC50 > 100 mg/L for D. subspicatus.

7.8.1.1. **Fish**

Short-term toxicity to fish

The toxicity of Florosa to *Oncorhynchus mykiss* was tested according to the OECD guideline 203, resulting in a 96h-LC50 of 354 mg/L. (unnamed report, 1989 - referred at the ECHA dissemination website). This information is taken into account as the most sensitive data on fish.

Long-term toxicity to fish

Data waived. No experimental study on long-term toxicity to fish is provided in the registration dossier.

7.8.1.2. **Aquatic invertebrates**

Short-term toxicity to aquatic invertebrates

An acute toxicity test on *Daphnia magna* performed according to OECD guideline 202 is provided by the registrants. An 48h-EC50 of ca. 320 mg/l was measured. The animals were exposed to the substance in a static test system (unnamed report, 1996 - referred at the ECHA dissemination website). This information is taken into account as the most sensitive data on aquatic invertebrate.

Long-term toxcicity to aquatic invertebrates

Data waived. No experimental study on long-term toxicity to aquatic invertebrates is provided by the registrants.

7.8.1.3. **Algae and aquatic plants**

The toxicity of the substance to algae was determined in a study according to the OECD guideline 201. The growth rate of the algae *Desmodesmus subspicatus* was investigated. After 72 hours an EC50 > 100 mg/l was indicated (unnamed report, 2006 - referred at the ECHA dissemination website). This information is taken into account as the most sensitive data on algae and is the basis for the derivation of the PNEC.

No long-term value is provided for algae in the registration dossier.

7.8.1.4. **Sediment organisms**

No study available.

7.8.1.5. **Other aquatic organisms**

No study available.

7.8.2. Terrestrial compartment

Data waived. No study is provided by the registrants on soil macroorganisms, terrestrial plants, soil microorganisms or other terrestrial organisms.

The substance is not readily biodegradable. However, as the log Koc is below 3 and the substance has no cationic properties, a low adsorption potential is indicated. Therefore, binding to sewage sludge is unlikely and as a consequence a transfer to the soil compartment is not expected.

7.8.3. Microbiological activity in sewage treatment systems

One study on the toxicity of 2H-pyran-4-ol on activated sludge is available in compliance with OECD guideline 209. An EC50 >1000 mg/L was determined after 180 minutes of incubation (unnamed report, 2007 - referred at the ECHA dissemination website). This information is taken into account for the derivation of the PNEC for microorganisms.

7.8.4. PNEC derivation and other hazard conclusions

According to the available information the substance was not classified for the environment. It was considered that the refinement of the exposure assessment will be enough to remove the initial concerns identified under the CoRAP. Therefore, the PNECs have been derived based on the short-term toxicity data initially provided by the registrants.

In the next table are compiled the ecotoxicological data selected for the PNEC derivation.

Table 10. Summary of the ecotoxicity data considered for the assessment.

	Endpoint
Short-term toxicity to fish	96h-LC50 354 mg/L
Short-term toxicity to aquatic invertebrates	48h-EC50 > 320 mg/l
Algal inhibition	72h-ECr50 >100 mg/l
STP microorganisms	3h-EC50 >1000 mg/l

Table 11. PNECs derivations.

PNEC DERIVATION AND OTHER HAZARD CONCLUSIONS		
Hazard assessment conclusion for the environment compartment	**Hazard conclusion**	**Remarks/Justification**
Freshwater	Hazard assessment conclusion (freshwater): PNEC 0.1 mg/L	Assessment factor: 1000
Marine water	Hazard assessment conclusion (marine waters): PNEC 0.01 mg/L	Assessment factor: 10000
Intermittent releases to water	Hazard assessment conclusion (intermittent releases): PNEC 1.00 mg/L	Assessment factor: 100
Sediments (freshwater)	Hazard assessment conclusion (sediment freshwater): PNEC 0.412 mg/kg dw	Extrapolation method: partition coefficient due to lack of data.
Sediments (marine water)	Hazard assessment conclusion (sediment marine water): PNEC 0.0412 mg/kg dw	Extrapolation method: partition coefficient due to lack of data.
Sewage treatment plant	Hazard assessment conclusion (STP): PNEC 10 mg/L	Assessment factor: 100
Soil	Hazard assessment conclusion (soil): PNEC 0.0902 mg/kg w	Extrapolation method: partition coefficient due to lack of data.
Secondary poisoning	-	Due to the Log Pow, a significant accumulation in organisms is not expected.

7.9. Human Health hazard assessment

The eMSCA screened the human health relevant endpoints with respect to PBT/CMR, but no relevant findings were observed.

7.9.1. Conclusions of the human health hazard assessment and related classification and labelling

See 7.6.1.

7.10. Assessment of endocrine disrupting (ED) properties

The eMSCA screened the endocrine disrupting relevant endpoints, but no relevant findings were observed.

7.11. PBT and vPvB assessment

1) Persistence,

The substance is considered as not ready biodegradable (0-10% degradation after 28 d, under activated sludge, non-adapted OECD Guideline 301 B), therefore, without any additional information, poor biodegradation rates are expected in surface water.

According to the conclusions from section 7.7.1 on degradation, the substance has to be regarded as potentially persistent (P) or even very persistent (vP) in the environment.

2) Bioaccumulation and,

No experimental study on bioaccumulation is provided in the registration dossier.

According to the estimated BCF of 5.04, the mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; transtetrahydro-2-isobutyl-4-methylpyran-4-ol is regarded as non bioacumulative substance.

3) Toxicity

Only acute data on ecotoxicity is provided in the registration dossier, indicating low toxicity to the aquatic organisms. According to this information the substance was not classified for the environment.

Human Health endpoints have also been reviewed by the eMSCA, regarding those aspects considered relevant for the assessment of the secondary poisoning or potential PBT/CMR characteristics. No concern for T has been identified.

According to the reviewed information the mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; transtetrahydro-2-isobutyl-4-methylpyran-4-ol is regarded as non toxic for the environment.

4) Overall conclusion

Based on the available information the substance does not fulfill the PBT criteria.

7.12. Exposure assessment

7.12.1. Human health

Not relevant for this assessment.

7.12.2. Environment

The main objective of this assessment is to remove the initial identified concerns demonstrating an acceptable level of exposure for the environment.

The environmental assessment of the mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol has been carried out using the initial information provided in the registration dossier, default exposure values according to the CHESAR/EUSES models and specific exposure site information provided by registrants.

Therefore, to confirm the environmentally safe use of the substance, specific on-site information was requested: Operational Conditions (OC) (including specific environmental conditions) and/or, Risk Management Measures (RMM) and/or, release rate measurements under frequent and regular monitoring of releases to environmental compartments, such as:

1. Number of emission days per year or daily use at sites.
2. Confirmation on the existence of STP(s) in the production/formulation plants.
3. Information on the management of STP-sludge (i.e. incineration, agricultural soil application…), if any.
4. Information on the effluent discharge rate freshwater of the STP(s) or the plant (in case of no existence of STP).
5. River flow rate(s) in which effluents are discharged.
6. Release(s) time per year.
7. Release(s) fraction to water.
8. Release(s) fraction to soil.
9. Confirmation on the existence of releases to marine water compartment.

The substance is the colourless organic liquid with a floral odour, used as an odour agent in fragrance blends and perfumes, consumer products, such as fine fragrance, personal/home care products, fabric care and laundry products. The substance is manufactured in a closed system.

Tonnage information:

Assessed tonnage: in the range of 1000-10000 tonnes/year based on production and import.

Exposure scenarios (ES) have been assessed according to the registration dossier. Tonnages per year of each company are included in the Confidential Information Annex.

As it has been indicated, if no other specific information is provided, the base of the assessment are the EUSES model, EU default environmental conditions, IFRA emission escenarios and site specific information provided by some registrants.

7.12.2.1. **Aquatic compartment (incl. sediment)**

According to the new information on exposure and risk management measures , the following PECs have been calculated by the eMSCA for the aquatic compartment.

Table 12. PECs for the aquatic compartment.

Company	Process	Freshwater (mg/L)	Freshwater Sed. (mg/kg dw)	Marine water (mg/L)	Marine sediment (mg/kg dw)
Company 1	Production	0.003	0.005	0.002	0.002
	Form/Comp	0.003	0.004	0.000	0.000
	Private use	0.002	0.013	0.001	0.001
Company 2	Production	0.049	0.119	0.001	0.012
	Form/Comp	0.006	0.014	0.000	0.001
	Private use	0.002	0.013	0.001	0.001
Company 3	Production	0.456	0.627	0.046	0.063
	Form/Comp	0.116	0.160	0.012	0.016
	Private use	0.005	0.007	0.000	0.001
Company 4	Formulation	0.045	0.061	0.004	0.006
	Private use	0.004	0.005	0.000	0.000
Company 5	Production	0.046	0.064	0.005	0.006
	Form/Comp	0.014	0.019	0.001	0.002
	Private use	0.003	0.004	0.000	0.000

Form: Formulation; Comp: Compounding

7.12.2.2. **Terrestrial compartment**

According to the information on exposure provided by registrants, the following local PECs are calculated by the eMSCA for the terrestrial compartment.

Table 13. PECs for the terrestrial compartment.

Company	Process	Agricultural soil (mg/kg dw)
Company 1	Production	0.003
	Form/Comp	0.001
	Private use	0.001
Company 2	Production	0.051
	Formulation	0.005
	Private use	0.001
Company 3	Production	0.076
	Form/Comp	0.019
	Private use	0.000

Company 4	Formulation	0.007
	Private use	0.000
Company 5	Production	0.007
	Form/Comp	0.002
	Private use	0.002

Form: Formulation; Comp: Compounding

7.12.2.3. **Atmospheric compartment**

-

7.12.3. Combined exposure assessment

-

7.13. Risk characterisation

Based on the available information the eMCSA concluded that "no classification" for the environment is justified. Initial grounds of concern regarding RCRs > 1 for some of the registrants have been removed. Estimated RCRs are included in the next table.

Table 14. RCRs calculated by the eMSCA for the aquatic compartment.

Company	Process	Freshwater (mg/L)	Freshwater Sed. (mg/kg dw)	Marine water (mg/L)	Marine sediment (mg/kg dw)
Company 1	Production	0.03	0.01	0.16	0.05
	Form/Comp	0.03	0.01	0.03	0.01
	Private use	0.03	0.01	0.03	0.09
Company 2	Production	0.49	0.29	0.11	0.29
	Form/Comp	0.06	0.03	0.06	0.03
	Private use	0.02	0.03	0.10	0.03
Company 3	Production	**4.56**	**1.52**	**4.56**	**1.52**
	Form/Comp	**1.16**	0.39	1.16	0.39
	Private use	0.05	0.02	0.05	0.02
Company 4	Formulation	0.45	0.15	0.45	0.15
	Private use	0.04	0.01	0.04	0.01
Company 5	Production	0.46	0.15	0.46	0.15
	Form/Comp	0.14	0.05	0.14	0.05
	Private use	0.03	0.01	0.03	0.01

Only the Company 3, which did not provided additional exposure information, results in RCRs slightly above 1. These ratios can be minimised considering the low aquatic short-term toxicity of the substance, which is in the range of 100-400 mg/L. Considering a factor of 10 to extrapolate from acute to chronic data, those RCRs slightly above 1 for the Company 3 would also be reduced to an acceptable risk below 1. Therefore, the risk for the aquatic compartment can be considered as acceptable.

ECOSAR estimates a ChV (96h) of 27.46 mg/L for fish, ChV (48h) of 14.30 mg/L for daphnid and a ChV of 14.30 mg/L for algae. The ChV, or Chronic Value in ECOSAR, is defined as the geometric mean of the no observed effect concentration (NOEC) and the lowest observed effect concentration (LOEC). So, it could be expected that the real NOECs will be a little bit lower than the estimated value. Considering these long-term values acceptable environmental RCRs will be acceptable for the Production and Formulation/Compounding scenarios of Company 3.

The risks associated to wide dispersive uses (private use) of the substance have also been clarified and considered acceptable (RCRs<1).

Tab 16. RCRs calculated by the eMSCA for the terrestrial compartment.

Company	**Process**	**Agricultural soil (mg/kg dw)**
Company 1	Production	0.03
	Form/Comp	0.01
	Private use	0.01
Company 2	Production	0.57
	Formulation	0.06
	Private use	0.01
Company 3	Production	0.84
	Form/Comp	0.22
	Private use	0.00
Company 4	Formulation	0.08
	Private use	0.00
Company 5	Production	0.08
	Form/Comp	0.02
	Private use	0.02

Therefore, after consideration of the exposure refinement carried out by the eMSCA it was concluded that there is no need for further actions or risk management measures to be implemented.

7.14. References

CHESAR, 2015. CHEmical Safety Assessment and Reporting tool. *https://chesar.echa.europa.eu/*

ECHA dissemination website (2015). Information on Chemicals (EC Nº 405-040-6). https://echa.europa.eu/substance-information/-/substanceinfo/100.100.664#IUPAC_NAMEScontainer (last revision, 2017)

EPISUITE4.11, 2015. U.S. Environmental Protection Agency for EPI SuiteTM. 2000 – 2012. *http://www.epa.gov/opptintr/exposure/pubs/episuitedl.htm*

EUSES 2.1. The European Union System for the Evaluation of Substances. https://ec.europa.eu/jrc/en/scientific-tool/european-union-system-evaluation-substances

IFRA, 2012. REACH Exposure Scenarios for Fragrance Substances. International Fragance Assotiation. *http://www.ifraorg.org/*

7.15. Abbreviations

CLP	Classification, Labelling and Package
CMR	Carcinogenic, Mutagenic and Reprotoxic
ECHA	European Chemicals Agency
eMSCA	Evaluating Member State Competent Authority
ERC	Exposure Release Category
EU	European Union
EUSES	European Union System for the Evaluation of Substances
IBCs	Intermediate Bulk Containers
IFRA	International Fregance AssociationOC Operational Contitions
PBT	Persistent, Bioaccumulable and Toxic
PEC	Prtedicted Environmental Concentration
RCR	Risk Characterization Ratio
RMM	Risk Management Measures
STP	Sewage Treatment Plant
vPvB	very Persistent, very Bioaccumulable