SUBSTANCE EVALUATION CONCLUSION

as required by REACH Article 48

and

EVALUATION REPORT

for

Quaternary ammonium compounds, tri-C8-10-alkylmethyl, chlorides

EC No. 264-120-7

CAS RN. 63393-96-4

Evaluating Member State: Italy

Date: 3 February 2023

Evaluating Member State Competent Authority

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Year of evaluation in CoRAP: 2017

Before concluding the substance evaluation, a Decision to request further information was issued on: 15 August 2019.

Further information on registered substances here:

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

DISCLAIMER

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. CONCERNS SUBJECT TO EVALUATION

The Substance, Quaternary ammonium compounds, tri-C8-10-alkylmethyl, chlorides was originally selected for substance evaluation to clarify concerns about:

- suspected PBT/vPvB
- wide dispersive use
- exposure to environment
- high RCR

2. OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

Up-to-date information on the activities planned, ongoing or completed on the Substance under REACH and CLP regulation can be found here:

https://echa.europa.eu/it/Quaternary ammonium compounds, tri-C8-10-alkylmethyl, chlorides

3. CONCLUSION OF SUBSTANCE EVALUATION

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

Table 1

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 (see explanation in Section B)

The current information does not allow to suggest any regulatory action at EU level.

The initial concerns were clarified. For details see sections below.

4. FOLLOW-UP AT EU LEVEL

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

Not applicable.

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 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.)	

This conclusion can be reached due to the outcome of the request of the eMSCA on physicochemical properties which suggest that the Substance does not screen as B and the exposure data shows no risk (see Part B).

5.2. Other actions

Not applicable.

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 Substance was originally selected for substance evaluation to clarify concerns about:

- suspected PBT/vPvB
- wide dispersive use
- exposure to environment
- high RCR

Table 3

EVALUATED ENDPOINTS	
Endpoint evaluated	**Outcome/conclusion**
Persistence	Concern unresolved. The Substance screens as P/vP. A simulation test to conclude the P assessment is not required according to the SEV decision since the Substance does not screen as B/vB based on the requested physico-chemical data.
Bioaccumulation	Concern inconclusive. The Substance does not screen as B/vB in aquatic organisms based on the requested physico-chemical data. Based on the currently available PBT guidance and the available data, the eMSCA cannot conclude on the bioaccumulation potential in air breathing organisms.
Toxicity	Concern unresolved.
Wide dispersive use Exposure to environment	Concern confirmed. Based on available information, further action not needed. For details see sections below.
High RCR	No concern, see section 7.13 below.

7.2. Procedure

The Substance evaluation was started in March 2017. The eMSCA considered that further information was required to clarify the PBT concerns. Therefore, it prepared a draft decision pursuant to Article 46(1) of REACH to request further information. It submitted the draft decision to ECHA on 21 March 2018. The Member State Committee reached a unanimous agreement on the draft decision in its MSC-65 written procedure and ECHA took the decision according to Article 52(2) and Article 51(6) of the REACH Regulation.

The following information was requested in a tiered strategy:

1. Solubility in pure n-octanol at 20°C:
   CIPAC method MT 181 (solubility in Organic Solvents) or OECD TG 105 (Water Solubility)
   and
   Critical micelle concentration in water (CMC) at 20°C. OECD TG 115 for surface tension measurements (Unconditionally)

2. Simulation study: OECD TG 309 (if results from tests 1 yield an estimated log K_{ow} higher than 4.5)

3. Bioaccumulation in Fish: Aqueous and Dietary Exposure: OECD TG 305 test (If results from test 2 show that the Substance fulfils the criteria for P or vP according to REACH Annex XIII (degradation half-life in fresh or estuarine water > 40 days)

Subsequently the Registrant(s) updated the dossier with information request 1, the first tier in the testing strategy. Following the assessment, the eMSCA concluded that no further action is needed.

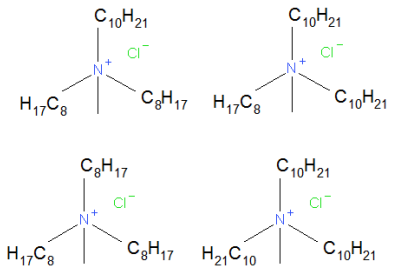
7.3. Identity of the substance

Table 4

SUBSTANCE IDENTITY	
Public name:	Quaternary ammonium compounds, tri-C8-10-alkylmethyl, chlorides
EC number:	264-120-7
CAS number:	63393-96-4
Index number in Annex VI of the CLP Regulation:	--
Molecular formula:	C8/C8/C8: C25H54N.Cl C8/C8/C10: C27H58N.Cl C8/C10/C10: C29H62N.Cl C10/C10/C10: C31H66N.Cl
Molecular weight range:	404.16-488.32 C8/C8/C8: 404.16 C8/C8/C10: 432.21 C8/C10/C10: 460.26 C10/C10/C10: 488.32
Synonyms:	--

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

Structural formulae:



The above structural formulae (clockwise) refer to individual substance constituents: C8/C8/C10, C8/C10/C10, C10/C10/C10 and C8/C8/C8, respectively.

Multi-constituent substance
The Substance was registered as a multi-constituent substance, with four main constituents that are structurally related and only differ by the lengths of the linear alkyl chains (C8 or C10). The Substance is a cationic surfactant. Nonetheless, the Substance is considered by the eMSCA as an UVCB oleochemical, due to the variability in the carbon chain length distribution.

Molecular formulae and molecular weights are indicated in the above Table for those chain lengths that, according to the qualitative/quantitative criteria under OECD TG 193 (*OECD guidance for characterising oleochemical substances for assessment purposes*), should be considered for the characterisation of this type of substance and included in the alkyl descriptor in the substance name.

Table 5

Constituents	Typical concentration	Concentration range	Remarks
methyltrioctylammonium chloride (C25H54N.Cl) EC/List no.: 225-896-2 CAS RN.: 5137-55-3	Confidential information	Confidential information	--
decylmethyldioctylammonium chloride (C27H58N.Cl) EC/List no.: --	Confidential information	Confidential information	--
didecylmethyloctylammonium chloride (C29H62N.Cl) EC/List no.: --	Confidential information	Confidential information	--
tridecylmethylammonium chloride (C31H66N.Cl) EC no/List.: -- CAS RN: 5137-56-4	Confidential information	Confidential information	--

7.4. Physico-chemical properties

The Substance is an oleochemical, where the four main constituents are structurally related and only differ by the lengths of their linear alkyl chains (C8 or C10). Therefore, they are expected to have similar behaviour and physico-chemical properties. As a result, the physicochemical endpoints have not been addressed separately for the individual constituents but the 'whole substance' approach has been used.

Table 6

OVERVIEW OF PHYSICOCHEMICAL PROPERTIES	
Property	**Value**
Physical state at 20°C and 101.3 kPa	Clear yellow to brown viscous liquid.
Vapour pressure	0.012 Pa at 20°C 0.020 Pa at 25°C (OECD Guideline 104, thermogravimetry)
Water solubility	1023 mg/L at 20°C (pH range: 3.8-4.4) (OECD Guideline 105, flask method; the test item concentration in the solutions was analysed by DOC, dissolved organic carbon analysis)
Partition coefficient *n*-octanol/water (Log K_{ow})	Log K_{ow}=3.9 (calculated by eMSCA considering a worst-case interpretation of the results). The K_{ow} was derived as the ratio of solubility in pure *n*-octanol at 20°C, i.e., 869 g/L or higher (1000 g/L), and critical micelle concentration (CMC) at 20°C

	as solubility limit in water (135.4 mg/L). Please, refer to eMSCA comments below.
Viscosity	Dynamic viscosity: 1985 mPa s at 20°C 488 mPa s at 40°C (OECD Guideline 114, rolling ball viscometer)
Flammability	The flammability of a liquid is established based on the flash point (and the boiling point). Based on the experience in the manufacturing, handling and use of the Substance, no pyrophoric properties are expected; the Substance does not liberate flammable gases on contact with water, either - not a flammable liquid - no pyrophoric properties - no flammability in contact with water
Flash point	77°C (closed-cup method using Pensky Martens apparatus according to DIN EN ISO 2719)
Autoflammability / self-ignition temperature	Auto-ignition temperature: 250°C, at 1013hPa (Regulation (EC) No 440/2008, A.15)
Explosive properties	Not explosive. No chemical groups associated with explosive properties are present in the chemical structure of the constituents
Oxidising properties	Not an oxidising liquid. No chemical groups associated with oxidizing properties are present in the chemical structure of the constituents
Granulometry	Not applicable, the Substance is a liquid
Stability in organic solvents and identity of relevant degradation products	The stability of the Substance is not considered to be critical
Dissociation constant	Not applicable. The Substance (salt) is irreversibly ionized. It does not possess any acidic or basic group, either
Melting / freezing point	Melting range: -5.2 to -0.4 °C (OECD Guideline 102, capillary method)
Boiling point	Boiling at >158°C under decomposition (OECD Guideline 103, capillary method)
Relative density	D^{20}_4 = 0.89 (OECD Guideline 109; pycnometer method)
Surface tension	27 mN/m at 20°C; test item concentration: 90% of saturation solubility, i.e., 993 mg/L (OECD Guideline 115, ring)
Solubility in octanol	869 g/L at 20°C (visual method) See further discussion below
Critical micelle concentration (CMC)	CMC 1 (0.1 mg/L to 1000 mg/L): 135.4 mg/L at 20°C (OECD TG 115) CMC 2 (1 mg/L to 1000 mg/L): 167.5 mg/L at 20°C (OECD TG 115) See further discussion below

Partition coefficient *n*-octanol/water (Log K_{ow}): eMSCA discussion

The Substance is an oleochemical, where the four main constituents are structurally related and only differ by the lengths of their linear alkyl chains (C8 or C10). Therefore, they are

expected to have similar behaviour and physical-chemical properties. As a result, the Kow derivation has not been carried out separately for the individual constituents but the 'whole substance' approach has been used.

The *n*-octanol/water partition coefficient (Kow) is necessary as a first step to clarify the B property of the Substance. No experimental results are available, since neither the Shake Flask Method nor the HPLC Method are applicable to surface-active materials, such as the Substance (surface tension: 27.0 mN/m at 20°C, determined according to OECD TG 115 by the ring method at 90% of saturation in water, i.e., 993 mg/L).

As an alternative to experimental testing, the Kow was originally covered by the Registrant(s) by QSAR calculations, performed by KOWWIN (v1.68) of EPI Suite v.4.11. The Log K_{ow} values of the individual quaternary ammonium constituents turned out to be in range 6.1 to 9.1, based on calculated values of water solubility (in the range 0.0016–0.000015 mg/L for the individual quaternary ammonium constituents). A second estimation was also carried out by the Registrant(s), using the experimental water solubility value of the Substance (1023 mg/L at 20°C, determined according to OECD TG 105 by the Flask Method). The re-calculated Log K_{ow} values submitted by the Registrant(s) proved to be very different, in the range from -0.094 to 0.52.

Nevertheless, the eMSCA is of the opinion that the Log K_{ow} prediction by KOWWIN should be regarded as inaccurate in any case, since the software database is limited for surfactants, mainly due to the lack of reference substances like the Substance of interest for validation purposes.

Additionally, the eMSCA is aware of some preliminary results from COSMOmic on one quaternary ammonium constituent, i.e., methyltrioctylammonium chloride, which suggest a lipid-water Log K_{ow} of about 7.8.

The above considered, the eMSCA believes that the best way-forward for a realistic Kow estimation is the calculation based on the ratio of solubility in pure *n*-octanol (whose determination was therefore requested by the eMSCA) and solubility in water (already available in IUCLID dossier) measured under the same temperature conditions. Also, the Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.7a: Endpoint specific guidance (Version 6.0, July 2017) considers a Kow calculation based on the measured *n*-octanol and water solubilities as the first choice for surfactants. CIPAC MT 181 can be used for testing. For solubilities below 10 g/L or for higher precision, OECD TG 105 (Water Solubility) may also be adapted.

The Guidance also suggests it might be prudent to take the critical micelle concentration in water (CMC) as a solubility limit, to avoid the artefact of unrealistically low Log K_{ow} values. OECD TG 115 shall be used for surface tension measurements.

Following the request of the eMSCA, the Registrant(s) determined the solubility in *n*-octanol. A preliminary test was conducted at room temperature (23°C) on a test item 98.3% pure. Results suggested a solubility in *n*-octanol of about 1000 g/L is to be expected for the Substance, and the 'flask method' in OECD TG 105 (fit for solubility $>10^{-2}$ g/L) should be followed. Nonetheless, practical limitations due to the physical state of the Substance (liquid) and its high solubility in *n*-octanol prevented the strict implementation of OECD TG 105. The preparation of saturated testing solutions is required by the 'flask method', but according to the Registrant(s) this is not feasible in case of liquid substances with high/complete miscibility with the solvent, such as the test item. As a result, an in-house method was applied: again, the test item and *n*-octanol were mixed at different ratios at room temperature (23°C). Testing solutions were then conditioned at (20.0±0.5) °C and visually checked for any phase separation. Complete miscibility of the two phases was observed up to a ratio of 99:1 (corresponding to 118 g test item in 0.11 g *n*-octanol, which is the maximum amount of test item dissolved in *n*-octanol to give a clear homogeneous solution). A solubility of 869 g test item/L or higher can be concluded.

As requested, CMC in water has been also derived, by measuring the surface tension of the test item solutions in water at increasing concentrations (OECD TG 115, ring method) and plotting the measured values versus the test item concentration in water. Since small plateau were observed at very low concentrations (below the proposed CMC of 135.4 mg/L), the Registrant(s) have been invited to further investigate the preliminary formation of micelles at very low-test item concentrations. NMR experiments at different test item concentrations (10-1100 mg/L) were additionally performed by the Registrant(s), which did not bring specific clarity on the issue, but confirmed the conclusions from the original CMC study. The Registrant(s) also referred to some literature data [Gyenge and Oloman, 2001], indicating a CMC in water of 1.4 x 10^{-4} mol/L at 25°C, roughly corresponding to 62 mg test item/L.

Once the solubility in octanol and the CMC have been measured, the Kow can be derived as their ratio. The result was compared with the B/vB screening criterion of Log K_{ow} > 4.5 (ECHA Guidance on Information Requirements and Chemical Safety Assessment Chapter R.11: PBT/vPvB assessment, Version 3.0, June 2017).

Considering a worst-case interpretation of the results, with a solubility in *n*-octanol of 869 g/L or higher (roughly 1000 g/L) and a CMC of 135.4 mg/L, a K_{ow} of 7.4 x 10^3 can be derived, corresponding to a Log K_{ow} of 3.9. Even opting for the CMC value from literature of 62 mg/L, the Log K_{ow} would still prove < 4.5 (Kow = 1.6 x 10^4, Log K_{ow} = 4.2).

All in all, the eMSCA considers that the B screening value of Log K_{ow} >4.5 is not met.
The eMSCA notes that ECHA Guidance on PBT/vPvB assessment is currently being updated (Chapter R.7c and R.11 of the Guidance on Information Requirements and Chemical Safety Assessment) and will include further guidance on the B assessment of surface active and ionisable substances. In addition, REACH Annex IX section 9.3.2 was updated in January 2022, 3 years after the SEV decision was sent. REACH Annex IX now states that it is not possible to waive the bioaccumulation test in aquatic species based on low Log K_{ow} if the Substance is ionisable or surface active at environmental pH, as this substance is. The conclusion that the Substance does not meet the B screening value is based on the scientific knowledge in 2019. Therefore, while the requested information does not support a concern, a bioaccumulation potential of the Substance cannot be fully excluded based on low Log K_{ow} alone.

7.5. Manufacture and uses

7.5.1. Quantities

Table 7

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 manufactured and/or imported in the European Economic Area in 100 - 1 000 tonnes per year and is used in formulation or re-packing and at industrial sites.

Formulation or re-packing
The Substance is used in the following products: pH regulators and water treatment products. Release to the environment of the Substance can occur from industrial use: formulation of mixtures.

Uses at industrial sites
The Substance is used for the manufacture of chemicals. It has an industrial use resulting in manufacture of another substance (use of intermediates). It is also used in the following areas: formulation of mixtures and/or re-packaging and mining. Release to the environment of the Substance can occur from industrial use: in processing aids at industrial sites, as processing aid and as an intermediate step in further manufacturing of another substance (use of intermediates).

Table 8

USES	Use(s)
Uses as intermediate	--
Formulation	Mixing or blending in (closed) batch processes for formulation of preparations – ERC2 (formulation of preparations)
Uses at industrial sites	Catalyst use Recycling – ERC4 (industrial use of processing aids in processes and products, not becoming part of articles) and ERC6B (industrial use of reactive processing aids).
Uses by professional workers	--
Consumer Uses	--
Article service life	--

7.6. Classification and Labelling

7.6.1. Harmonised Classification (Annex VI of CLP)

The Substance is not currently listed in Annex VI of CLP Regulation ((EC) No 1272/2008).

7.6.2. Self-classification

- In the registration(s):

Containing >= 0.3 % but < 1 % of CAS RN 68814-95-9
Acute Tox. 3 H301
Skin Corr. 1C H314
Eye Damage 1 H318
Repr. 1B H360
Aquatic Acute 1 H400
Aquatic Chronic 1 H410

Containing > 1 % but <= 2 % of CAS RN 68814-95-9
Acute Tox. 3 H301
Skin Corr. 1C H314
Eye Damage 1 H318
Repr. 1B H360
STOT Rep. Exp. 2 (heart) H373
Aquatic Acute 1 H400

Aquatic Chronic 1 H410

Containing < 0.3 % of CAS RN 68814-95-9
Acute Tox. 3 H301
Skin Corr. 1C H314
Eye Damage 1 H318
Repr. 2 H361
Aquatic Acute 1 H400
Aquatic Chronic 1 H410

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

Acute Tox. 4 H302
Skin Irrit. 2 H315
Skin Corr. 1B H314

7.7. Environmental fate properties

7.7.1. Degradation

The Substance and its substructures do not contain hydrolysis sensitive structures.

No relevant information is available regarding phototransformation in air, in water and in soil.

Regarding screening tests on biodegradation in water, the Registrant(s) provided a ready biodegradability study (Unpublished, 2013, Registration dossier) conducted according to a standard test protocol (OECD TG 301D, Ready biodegradability Closed Bottle test) and in compliance with GLP. The study was performed on the Substance. After 28 d, no biodegradation was observed (-3%) whereas after a test prolongation up to 60 days a slight biodegradation activity of 10-20% was observed. The Registrant(s) concluded that the Substance is neither readily biodegradable nor inherently biodegradable and, based on the available information, the eMSCA can support this conclusion.

Biowin models (v. 4.10) were used by the Registrant(s) to screen if the Substance potentially fulfils criteria for ready biodegradability and persistence. In the six models for aerobic degradation prediction the criteria for fast degradation were met, while the result of Biowin 7 (Anaerobic Model Prediction) was the Substance does not biodegrade fast. The three estimation models Biowin 2 (non-linear model prediction), Biowin 3 (ultimate biodegradation time) and Biowin 6 (MITI non-linear model) were also used to screen the Substance for criteria of persistence, as suggested by the ECHA Guidance on Information requirements and chemical safety assessment R11. The combined results of Biowin 2 (0.94), 3 (3.2) and 6 (0.55) do not fulfil the reported criteria in Table R.11-4 of the ECHA guidance to screen the Substance as potential P/vP.

The eMSCA highlights that although the molecular weight of the Substance is in the range of the training set compounds for the models Biowin 2 and 3, the functional group quaternary ammonium is not represented in the training set of both models. In addition, the Biowin models 2 and 3 recognise only the linear C4 terminal chain fragments. Therefore, not all the carbon atoms are included in the recognized fragments in the Biowin 2 and 3 predictions. In Biowin 6 all the carbon atoms as well as the quaternary amine are covered by the recognised fragments. Biowin 6 recognises the alkyl chains as 21 -CH2- [linear] fragments. This fragment has a positive coefficient in the model. It should be noted that Biowin models multiply the coefficient for each of the fragments by the number of the fragment and therefore, in the case of a positive fragment coefficient, may overestimate biodegradation because any possible negative effect due to increased number of fragments (such as steric factors) are not considered (further details are available in BIOWIN User's Guide (v 4.10), 9.0. Known Problems with Biowin models (Biowin 1-7)).

Thus, it is possible that the Biowin 6 result overestimates the biodegradation in this case. The eMSCA concludes that the Substance is not readily biodegradable, based on the results of the prolonged ready biodegradability test.

No relevant information is available regarding water, sediment, and soil simulation tests.

7.7.2. Environmental distribution

The study on adsorption/desorption was waived by the Registrant(s) since the calculated Log K_{ow} was in the range of –0.094 and 0.52 for the individual quaternary ammonium constituents of the Substance. These values were used by the Registrant(s) to calculate Log K_{oc} for the individual constituents by KOCWIN vs 2.0. The result was Log K_{oc} values in the range 0.78-1.12. The value of 0.78 was used by the Registrant(s) in the PNEC sediment and soil calculation.

The eMSCA considers that the estimation of Koc, based on Log K_{ow} calculated using KOWWIN, is not reliable as the software database is not so representative of surfactants. Moreover, as input, Registrant(s) used the estimated values of Kow referred to individual constituents, instead of the updated values referred to the whole substance.

Since the Substance is a surfactant, Kow value is likely to be poor predictor of adsorption of this type of substances.

For the above-mentioned reasons, the Log K_{oc} value of 0.78 is considered not reliable by the eMSCA.

No information about volatilisation and distribution modelling is available in the registration dossier.

7.7.3. Bioaccumulation

The results were initially evaluated by Registrant(s) in a weight-of-evidence approach from QSAR estimations, read-across information, and DiamMax-Average arguments.

Considering the new information provided by the Registrant(s), a Log K_{ow} value of 3.9 has been determined, based on the most conservative outcome derived from the separate measurement of the Substance solubility in *n*-octanol and its CMC in water. Based on this, the eMSCA concludes that the Log K_{ow} of the Substance (< 4.5) does not fulfil the screening criteria for aquatic bioaccumulation.

The eMSCA notes that ECHA Guidance on PBT/vPvB assessment is currently being updated (Chapter R.7c and R.11 of the Guidance on Information Requirements and Chemical Safety Assessment) and will include further guidance on the B assessment of surface active and ionisable substances. In addition, REACH Annex IX section 9.3.2 was updated in January 2022, 3 years after the SEV decision was sent. REACH Annex IX now states that it is not possible to waive the bioaccumulation test in aquatic species based on low Log K_{ow} if the Substance is ionisable or surface active at environmental pH, as this substance is. The conclusion that the Substance does not meet the B screening value is based on the scientific knowledge in 2019. Therefore, while the requested information does not support a concern, a bioaccumulation potential of the Substance cannot be fully excluded based on low Log K_{ow} alone.

The eMSCA notes that no information on the log KOA of the Substance was available. QSAR predictions by KOAWIN (v1.10) were used to estimate the log KOA value (range from 11.08 to 6.31), recognizing however the poor applicability of the model for surfactants. Nevertheless, in all the cases the estimates lead to a log KOA greater than 5, thus indicating that the Substance (potentially) fulfils the screening criteria (log K_{OW} >2 and log KOA >5) for bioaccumulation in air-breathing organisms. In absence of toxicokinetic data on mammals, we note that the octanol solubility of the Substance (869 g/L) greatly exceeds

the adjusted value of MW x 0.002 mM, which is an indication of a potential mass storage into lipid tissues of air-breathing organisms according to the R.11.4.1.2.11 of the Guidance on Information Requirements and Chemical Safety Assessment (ECHA, 2017). However, the eMSCA considers that the available information is not sufficient to conclude on whether the Substance bioaccumulates into air-breathers.

QSAR estimation

The eMSCA addressed various QSAR models to estimate the BCF of the Substance with the help of VEGA platform. These models were CAESAR (V. 2.1.14), Meylan (V. 1.0.3) and KNN/Read-Across (V. 1.1.0). In all the cases the estimated BCF was fairly below the threshold of 2000 L/Kg, but the predictions were affected by large uncertainties since the Substance fell outside the applicability domain of each model. For this reason, the eMSCA concludes that the BCF values obtained through QSAR predictions cannot be considered a reliable indicator of the Substance bioaccumulative potential.

Read-across information

For completeness, of the evaluation, the eMSCA has considered information regarding several studies on bioaccumulation reported from the EU risk assessment for substance dimethyldioctadecylammonium chloride (DODMAC, CAS RN 107-64-2) and Di(hydrogenated tallow alkyl)dimethylammonium chloride (DHTDMAC, CAS RN 61789-80-8), listed in the EU risk assessment (EURAR 2002, addendum 2009). DODMAC and DHTDMAC belong to the group of the quaternary ammonium compounds (QACs or quats) and are cationic surfactants.

DHTDMAC is a mixture of quaternary ammonium compounds, with DODMAC as the main component, which is produced from hardened, i.e., hydrogenated natural fats. The alkyl chain length distribution related to the total molecule in standard European products with bovine tallow as the most important raw fat (e.g., Praepagen WK, Genamin DSAC) is:
C12: max. 2%
C14: 1 - 5%
C16: 25 - 35%
C18: about 65%
C20: max. 2% (Hoechst AG, 1980)

According to these distributions, DHTDMAC consists of about 65% of C18-chains. Since each molecule contains two alkyl chains, the proportion of DODMAC related to the total content of dimethyldialkylammonium compounds can be estimated as 42% DODMAC contained in DHTDMAC.

Table 10. In the following table several studies on bioaccumulation are available reported from the above-mentioned EU risk assessment for DHTDMAC and DODMAC.

Fish	Substance	Type of water	Concentration	Suspended solids	Exposure time	BCF
Lepomis macrochirus	C14-DHTDMAC	River water	18 µg/L	2-84 mg/L	49 d	13 L/kg w.b. / 94 L/kg inedible tissue / <5 L/kg in fillet
Lepomis macrochirus	C14-DHTDMAC	Laboratory water	16 µg/L	--	49 d	32 L/kg w.b. / 256 L/kg inedible

						tissue
Pimephales promelas	DODMAC	Laboratory water	--	6.8 mg/L humic acid	24 h	humic acid decreased uptake rate by factor 20

Invertebrate	**Substance**	**Sediment**	**Concentration**	**Organic carbon**	**Exposure time**	**expressed as BSAF**
Lumbriculus variegatus	C14-DODMAC	natural sediment	150-5800 mg/kg dw	organic carbon of sediment 1.73%	28d	Biota sediment accumulation factor (BSAF): 0.28
Tubifex tubifex	C14-DODMAC	natural sediment	300-5000 mg/kg dw	organic carbon of sediment 1.73%	28d	Biota sediment accumulation factor: 0.78

The authors of the risk assessment highlighted a dependence of the BCF-values on the surrounding medium, which is also obvious in ecotoxicological testing. Based on test results with laboratory water, there is bioaccumulation, but it is assumed that it is low under actual environmental conditions.

Bioaccumulation studies in fish and sediment organisms cited in the risk assessment for DOMAC and DHTMAC, show a trend of a reduced bioaccumulation potential.

The eMSCA highlighted that these studies can be considered just as supporting information indicating that it is possible to perform aqueous BCF tests on substances cationic surfactants belonging to the group of the quaternary ammonium compounds. In general, QACs share the common quaternary ammonium cation. The substituents R1, R2, R3 and R4 are varied to influence the properties of the ion. In pure form the QACs will also contain an anion such as chloride, bromide or methosulfate. When in solution, like in a sewage system, the substances will be dissociated and the anion the QACs were once associated with will be irrelevant.

According to the literature report "Quaternary ammonium compounds Analyses in a Nordic cooperation on screening" (TemaNord 2014:556), quat cations of the types alkyltrimethylammonium (ATAC), alkyldimethylbenzyl (benzalkonium, BAC) and dialkyldimethylammonium (DDAC) were investigated. For the analysed quats, the compound properties vary with alkyl chain length. Water solubility decreases, and adsorptivity to surfaces increases, with increasing chain length.

Additional considerations by the eMSCA
In the updated registration dossier, the Registrant(s) provided a new Log K_{ow} value. An octanol solubility of 896 g/L at 20°C was measured through a method analogue to OECD TG 105. Two different methods were used to measure water solubility. In the first case an OECD TG 105 method was followed resulting in a value of 1023 mg/L at 20°C. In the second case, an OECD TG 115 was used to determine the CMC in water, leading to values of 135.4 mg/L and 167.5 mg/L. The eMSCA considers that the most conservative estimate of the Log K_{ow} derives from the ratio between the solubility of the Substance in octanol and the lowest value of its CMC in water. This corresponds to a Kow of 6.4×10^3 and therefore to a Log K_{ow}= 3.9.

7.8. Environmental hazard assessment

7.8.1. Aquatic compartment (including sediment)

7.8.1.1. Fish

Two short-term tests on fish are available in the registration dossier. One unreliable study, without GLP and no analytics, reports 96h LC_{50} in zebrafish 0.094 mg/L.

The second study on the short-term toxicity on fish, is considered by the Lead Registrant as reliable without restrictions (Unpublished, 2013 in Registration dossier). In the test, performed according to OECD TG 203 guideline, *Danio rerio* fish were exposed 96 h to the Substance. A 96h LC_{50} of 0.150 mg/L was determined. The nominal concentrations ranged from 0.105 to 0.300 mg/L, which were below the limit of quantification and the limit of detection of 2.50 and 1.25 mg/L, respectively. Consequently, no analytical measurement could be performed. Therefore, the test results were based on the nominal concentrations. Moreover, the test material resulted only partially soluble, and resulting water soluble fractions (WSF) were used in the test. In conclusion, no information on the effective concentrations were provided.

No available information on Long-term toxicity to fish.

7.8.1.2. Aquatic invertebrates

Short-term effects of the Substance were assessed on the freshwater cladoceran *Daphnia magna* according to the OECD TG 202 (*Daphnia sp.* Acute Immobilisation Test). The results showed:

- EC_{50} (48h): 0.16 mg/L test mat. (Nominal)
- EC_{10} (48h): 0.11 mg/L test mat. (nominal)

The eMSCA notes that nominal test concentrations (0.063 - 1 mg/L) were below the limits of quantification and detection of 2.50 and 1.25 mg/L, respectively; thus, the analytical verification of test concentrations could not be performed, and results were expressed as nominal loading rates. Still, the test material was only partially soluble, and water-soluble fractions (WSF) were used in the test.

Overall, the eMSCA considers this study as reliable with restriction based on the lack of analytical verification of test concentrations.

No information is available on long-term toxicity to aquatic invertebrates.

7.8.1.3. Algae and aquatic plants

A reliable experimental study (Unpublished, 2013b in Registration dossier), static on *Desmodesmus subspicatus*, performed with the Substance, according to OECD TG 201 (Alga, Growth Inhibition Test) and under GLP, is provided in the registration dossier.
A 72h ErC_{50} value of 0.29 mg/L (nominal) and a 72h ErC_{10}/NOEC of 0.138 mg/L (nominal) have been determined for the effects of the Substance on growth rate of algae.

The eMSCA considers study results to be reliable and suitable for the purpose of CSA.

7.8.1.4. Sediment organisms

No information available

7.8.2. Terrestrial compartment

No studies on the toxicity of the Substance to all three terrestrial taxonomic groups (soil macro-organisms, soil micro-organisms and terrestrial plants) are available.

According to ECHA Guidance R7.c, in absence of toxicity data for soil organisms, the Equilibrium Partitioning Method (EPM) has been applied to assess the hazard to soil organisms for the Substance. In this case, the screening risk assessment for the soil compartment based on EPM (including an additional safety factor of 10 applied) showed safe use for all exposure scenarios (with RCRs values for agricultural soil ≤0.01). Therefore, also considering the absence of risk (EPM based-screening assessment PEC/PNECsoil<<1

with additional safety factor of 10 applied), the eMSCA concludes that no hazard to soil organisms can be expected.

7.8.3. Microbiological activity in sewage treatment systems

The registration dossier contains a reliable test result conducted on the Substance indicating an EC50 (3h) =18 mg/L (based on nominal concentrations) and an EC10 (3h) =4.4 mg/L (based on nominal concentrations). The study, with reliability 1, was performed according to the OECD TG 209 (Activated Sludge, Respiration Inhibition Test) and under GLP. The activated sludge was incubated for 3 hours with nominal concentrations:

EC_{50} (3h) =18 mg/L
EC_{10} (3h) =4.4 mg/L

Based on the available information, the eMSCA can support the conclusion on this endpoint.

7.8.4. PNEC derivation and other hazard conclusions

PNEC values for the aquatic compartments is based on acute toxicity data. Lowest value is for fish (LC_{50} = 0.15 mg/L).

In the test, performed according to OECD TG 203, *Danio rerio* fish were exposed 96 h to the Substance. A LC_{50} of 0.150 mg/L was determined. This value was the lowest acute toxicity data from the three trophic levels and was used for the PNEC calculation and for the risk assessment in the CSR. The nominal concentrations ranged from 0.105 to 0.300 mg/L, which were below the limit of quantification and the limit of detection of 2.50 and 1.25 mg/L, respectively. Therefore, no analytical measurement could be performed. Therefore, the test results were based on the nominal concentrations. Moreover, the test material resulted only partially soluble, and resulting water soluble fractions (WSF) were used in the test. In conclusion, no information on the effective concentrations were provided.

In absence of any ecotoxicological data for terrestrial organisms, the PNEC soil was derived using the equilibrium partitioning method (EPM). The eMSCA highlights that, considering the above-mentioned critical issues related to the Log K_{oc} value used for CSA (see paragraph 7.7.2.), the value of PNEC soil as provided by the Registrant(s) could be revised. To sum up, following the outcome of CSA and considering the absence of risk (RCRs for soil ≤0.01) by using an EPM based-screening assessment PEC/PNECsoil<<1 with additional safety factor of 10 applied (in a worst-case approach according to R.10 ECHA Guidance), eMSCA agrees with Registrant(s) that the information available is sufficient to conclude on no concern for hazard to soil organisms.

The PNEC sediment also was derived using the equilibrium partitioning method (EPM). The eMSCA can support the Registrant(s)' approach however noting the same above-mentioned critical issues related to the Log K_{oc} value used for CSA (see paragraph 7.7.2.), the value of PNEC sediment as provided by the Registrant(s) could be revised.

Table 11

PNEC DERIVATION AND OTHER HAZARD CONCLUSIONS		
Hazard assessment conclusion for the environment compartment	**Hazard conclusion**	**Remarks/Justification**
Freshwater	PNEC freshwater: 0.00015 mg/L	Assessment factor: 1000 Extrapolation method: assessment factor

Marine water	PNEC marine water: 0.000015 mg/L	Assessment factor: 10000 Extrapolation method: assessment factor
Intermittent releases to water	PNEC intermittent releases: 0.0015 mg/L	Assessment factor: 100 Extrapolation method: assessment factor
Sediments (freshwater)	PNEC sediment (freshwater): 0.055 mg/kg sediment dw	Extrapolation method: EPM eMSCA note: Log K_{oc} value shows some critical issue. PNEC calculation could be revised (see above)
Sediments (marine water)	PNEC sediment: 0.005 mg/kg sediment dw	Extrapolation method: EPM eMSCA note: Log K_{oc} value shows some critical issue. PNEC calculation could be revised (see above)
Sewage treatment plant	PNECSTP: 0.44 mg/L	Assessment factor: 10 Extrapolation method: assessment factor
Soil	PNEC soil = 38 ng/kg soil dw	Extrapolation method: EPM No toxicity data for soil organisms are available and no exposure to soil is expected. The PNEC soil value was derived using EPM, with default values. eMSCA can support the soil hazard assessment conclusions, including the EPM-based PNEC soil derivation. However, eMSCA notes that, considering the above-mentioned critical issues related to the Log K_{oc} value used for CSA (see paragraph 7.7.2.), the value of PNEC soil as provided by the Registrant(s) could be revised (see above).
Air	No hazard identified	--
Secondary poisoning	(Not evaluated) PNEC oral: 1.66 mg/kg food	--

7.8.5. Conclusions for classification and labelling

The Substance is considered not rapidly biodegradable and with low potential for bioaccumulation. The lowest value of acute toxicity is 0.15 mg/L. The only value of chronic toxicity obtained with algae is EC_{10} = 0.138 mg/L.

Acute Toxicity: Aq. Acute 1, H400, M = 10
Discussion by the eMSCA: M-factor acute should be 1 due to the lowest value for the acute toxicity.

Chronic Toxicity: Aq. Chronic 1, H410
The chronic classification is based on the values for acute toxicity.
Discussion by the eMSCA: M-factor chronic should be 1 due to the lowest value for the acute toxicity.

7.9. Human Health hazard assessment

7.9.1. Toxicokinetics

Not evaluated.

7.9.2. Acute toxicity and Corrosion/Irritation

Not evaluated.

7.9.3. Sensitisation

Not evaluated.

7.9.4. Repeated dose toxicity

Not evaluated.

7.9.5. Mutagenicity

Not evaluated.

7.9.6. Carcinogenicity

Not evaluated.

7.9.7. Toxicity to reproduction (effects on fertility and developmental toxicity)

Not evaluated.

7.9.8. Hazard assessment of physico-chemical properties

None impacting human health.

7.9.9. Selection of the critical DNEL(s)/DMEL(s) and/or qualitative/semi-quantitative descriptors for critical health effects

Not relevant for this evaluation.

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

Not evaluated.

7.10. Assessment of endocrine disrupting (ED) properties

Not evaluated.

7.11. PBT and vPvB assessment

The Substance consists of four constituents whose chemical structures are very similar. They differ only by the length of the alkyl chain substituents (C8 or C10). The eMSCA considers that the physico-chemical and PBT properties of each constituent will be very similar due to their similar structures. They are expected to have a similar mode of action for aquatic toxicity.

1) Persistence

Concerning abiotic degradation, the Substance does not contain hydrolysis sensitive structures.
No relevant information is available regarding phototransformation in air, in water and in soil.

Regarding screening tests on biodegradation in water, the Registrant(s) provided a ready biodegradability study (Unpublished, 2013 in Registration dossier) conducted according to a standard test protocol (OECD TG 301D, Ready biodegradability Closed Bottle test) and in compliance with GLP. The study was performed on the Substance. After 28 d no biodegradation was observed (-3%) whereas after a test prolongation up to 60 days a slight biodegradation activity of 10-20% was observed. The eMSCA concludes that the Substance is neither readily biodegradable nor inherently biodegradable based on the available information. The Substance screens as P/vP.

Additional modelling using Biowin 1-7 by Biowin vs. 4.10 was performed with the test item to screen if the Substance potentially fulfils criteria for P. The combined results of Biowin 2 (0.94), 3 (3.2) and 6 (0.55) do not fulfil the criteria reported in ECHA Guidance on Information requirements and chemical safety assessment R11, Table R.11-4., suggesting that the Substance does not screen as persistent.

The eMSCA highlights that although the molecular weight of the Substance is in the range of the training set compounds for the models Biowin 2 and 3, the functional group quaternary ammonium is not represented in the training set of both models. In addition, the Biowin models 2 and 3 recognise only the linear C4 terminal chain fragments. Therefore, not all the carbon atoms are included in the recognized fragments in the Biowin 2 and 3 predictions. In Biowin 6 all the carbon atoms as well as the quaternary amine are covered by the recognised fragments. Biowin 6 recognises the alkyl chains as 21 -CH2- [linear] fragments. This fragment has a positive coefficient in the model. It should be noted that Biowin models multiply the coefficient for each of the fragments by the number of the fragment and therefore, in the case of a positive fragment coefficient, may overestimate biodegradation because any possible negative effect due to increased number of fragments (such as steric factors) are not considered (further details are available in BIOWIN User's Guide (v 4.10), 9.0. Known Problems with Biowin models (Biowin 1-7)).

Thus, it is possible that the Biowin 6 result overestimates the biodegradation in this case. Since the Biowin 6 prediction (0.55) is close to the cut-off value and due the limitations in the Biowin predictions, the eMSCA considers that the fact the Biowin screening criteria are not fulfilled does not support that the Substance is not P or vP.

No relevant information is available regarding water, sediment, and soil simulation tests.

Conclusion: Based on the results of the Ready biodegradability Closed Bottle test, the Substance is considered as potential P/vP. Further information and potentially further assessment on persistency of the Substance would be necessary to reach a definite conclusion. The OECD TG 309 was requested in the SEV decision in a tiered strategy. Since the Substance is concluded not to screen as B/vB, the OECD TG 309 study is not required according to the tiered strategy.

2) Bioaccumulation

Based on the new data provided by the Registrant(s), the Substance has a Log K_{ow} of 3.9. Based on this, the eMSCA concludes that the Substance does not fulfil the screening criteria for aquatic bioaccumulation (Log K_{ow} <4.5). Also, no further assessment is deemed necessary since the BCF determination in a fish study (OECD 305 test, under Request 3) was conditional to the confirmation of the P/vP properties of the Substance through an OECD 309 study, which in turn was conditional to the occurrence of a Log K_{ow} >4.5.

The eMSCA addressed various QSAR models to estimate the BCF of the Substance with the help of VEGA platform. These models were CAESAR (V. 2.1.14), Meylan (V. 1.0.3) and KNN/Read-Across (V. 1.1.0). In all the cases the estimated BCF was below the threshold of 2000 L/Kg, but the predictions were affected by large uncertainties since the Substance fell outside the applicability domain of each model.

BCF studies for the structurally related substances dimethyldioctadecylammonium chloride (DODMAC, CAS RN 107-64-2) and Di(hydrogenated tallow alkyl)dimethylammonium chloride (DHTDMAC, CAS RN 61789-80-8), can be used as supporting information: *Lepomis macrochirus* BCF 32; *Tubifex* BSAF 0.78.

Conclusion: The Substance does not fulfill the screening criteria for aquatic bioaccumulation. No further assessment in aquatic vertebrates is necessary. The eMSCA notes that ECHA Guidance on PBT/vPvB assessment is currently being updated (Chapter R.7c and R.11 of the Guidance on Information Requirements and Chemical Safety Assessment) and will include further guidance on the B assessment of surface active and ionisable substances. In addition, REACH Annex IX section 9.3.2 was updated in January

2022, 3 years after the SEV decision was sent. REACH Annex IX now states that it is not possible to waive the bioaccumulation test in aquatic species based on low Log K_{ow} if the Substance is ionisable or surface active at environmental pH, as this substance is. The conclusion that the Substance does not meet the B screening value is based on the scientific knowledge in 2019. Therefore, while the requested information does not support a concern, a bioaccumulation potential of the Substance cannot be fully excluded based on low Log K_{ow} alone.

Apart from aquatic organisms, the eMSCA however notes that potential bioaccumulation in other organisms cannot be excluded.

For this reason, the B concern is inconclusive.

3) Toxicity

Environment

Fish:
Danio rerio: 96h-LC_{50} = 0.150 mg/L (nominal); (OECD TG 203) the water accommodated fraction (WAF) approach was used
No information on the effective concentrations were provided
Danio rerio: 96h-LC_{50} = 0.094 mg/L (nominal); (equivalent or similar to ISO 7346-1, Ref. Göran D. et al.1981). Considered Not Reliable

Invertebrates
Daphnia magna: 48h-EC_{50} = 0.16 mg/L (nom) (OECD TG 202)

Algae
Desmodesmus subspicatus: (OECD TG 201) results based on: growth rate
72h-EC_{50} = 0.29 mg/L (nominal)
72h-EC_{10} = 0.138 mg/L (nominal)
The provided EC_{10} for algae is > 0.01 mg/L.

Based on the acute aquatic ecotoxicity studies, there is no indication of T, but no definite conclusion can be reached, in the absence of long-term aquatic toxicity data on fish and invertebrates.

Human health
Self-classification:
Based on the available read-across data, no classification for toxicity to reproduction is necessary. If, however the content of CAS RN 68814-95-9 (self-classified as Repr. Cat. 1B, Fertility and Development) is at or greater than 0.3% (but less than 10%), a classification with Repr. Cat. 1B is warranted.

Based on the available read-across data, no classification for repeated dose toxicity is necessary. However, if the content of CAS RN 68814-95 -9 (STOT RE Cat. 1 for effects on the heart) is at or greater than 1% (but less than 10%), a classification with STOT RE Cat. 2 for potential effects on the heart is warranted.

However, the eMSCA concluded that according to available information, the whole substance could be considered fulfilling the T-criterion in accordance with Annex XIII, because as stated by Registrant(s), the Substance as a range 0-2%(w/w) of the impurities Amines CAS RN 68814-95-9, relevant for C&L.

4) Overall conclusion

P
The Substance is not readily biodegradable. Therefore, it should be deemed potential P/vP.

B

The provided information, while precluding a direct comparison with the Annex XIII criteria for B/vB substances, indicates that the Substance has a limited tendency to bioaccumulate into the aquatic organisms, based on the physico-chemical data.

According to the tiered testing strategy in the SEV decision, there is no need to generate further information and/or additional assessment on bioaccumulation of the Substance. The eMSCA notes that the conclusion that the Substance does not meet the B screening value is based on the scientific knowledge in 2019. However, the Substance potentially fulfils the screening criteria for bioaccumulation into air-breathers. Based on the currently available PBT guidance and the available data, the eMSCA therefore cannot conclude on the bioaccumulation potential into these organisms.

T
The Substance is self-classified by Registrant(s) Repr. cat 1B and STOT-RE cat. 2 criteria based on the presence of the impurity Amines, tri-C8-10-alkyl EC /List number: 272-347-8 in the concentration range 0.0-2.0% (w/w). However, T criterion is fulfilled based on the self-classified impurity. The Substance fulfills the T-criterion in accordance with Annex XIII for human health.

Based on the available information the Substance is potential P/vP, T, with inconclusive B. Therefore, the PBT/vPvB properties according to Annex XIII criteria cannot be confirmed.

7.12. Exposure assessment

7.12.1. Human health

Not evaluated.

7.12.2. Environment

According to information in the registration dossier and in the chemical safety report the Substance is used in pH regulators and water treatment products. Industrial use results in manufacture of another substance. At the workplace, closed batch processing in synthesis or formulation and mixing in open batch processes are reported.

The Registrant(s) stated that the exposure scenarios (9.1 to 9.3) have been calculated using EasyTRA 5.2.0; algorithms based on the latest versions of the ECHA REACH Guidance chapters R12, R14, R15, and R16 and EUSES®.

In contributing scenarios controlling environmental exposure, the Registrant(s) has applied default values for release factors taken from the environmental release categories (ERC) or refinements based on the available specific environmental release categories (SPERC - ECMA); at the same time were assumed refined release factor different to the default ones without providing complementary/additional source information and justifications as required by the ECHA Guide R.16.2.3.2.

Aquatic compartment (incl. sediment)
As stated in the supporting document provided by the Registrant(s), all reported RCR values in the exposure scenarios for industrial use and formulation of preparations are less than 1 and the risk is controlled in the aquatic environment.

For all scenarios, Simple Treat 4.0 has been used for modelling the biological sewage treatment plant (STP) according to ECHA Guidance on information requirements and Chemical Safety Assessment, Chapter R.16.

The eMSCA notes that the Registrant(s) applies a release factor other than the predefined ones (ERC-SPERC / ECMA) without providing complementary / additional information and justifications as required by ECHA guidance R.16.2.3.2.

Terrestrial compartment
The Registrant(s) states that for all scenarios, the sewage sludge is quantitatively incinerated (100%) and should not be applied to agricultural soil.

All reported RCR values calculated in the exposure scenarios for industrial and formulation use are less than 1 and the risk is controlled in this environmental compartment.

However, the eMSCA notes that in the updated CSR, it still applied the processing data for "Municipal" STP for the risk assessment calculations in all exposure scenarios. Also, it is noted that the municipal STP scenario does not warrant incineration as a risk management measure as it cannot be assumed that municipal STP facilities incinerate the sludge produced.

Atmospheric compartment
The Registrant(s) considered that the Substance is not considered to pose a hazard to the air for all three scenarios. However, the eMSCA notes that the Registrant(s) did not provide a clear supporting justification.

Combined exposure assessment
The Registrant(s) provided the regional predicted environmental concentration (PEC regional), the Predicted exposure concentrations and risks for the environment and man via the environment due to all widespread uses, and the related risk characterisation ratios. The exposure estimates have been obtained utilizing the SimpleBox Model as proposed by the TGD while local emissions at the STP were calculated using the formulae given in the TGD.

Secondary poisoning considers indirect exposure of man via foods, air and drinking water. It is calculated by identifying the exposure of the Substance from exemplary food sources at different trophic levels together with the total exposure on all food routes and sources. The environmental exposure calculation per compartment is based on the algorithms of the EU TGD 2003 Risk Assessment Spreadsheet Model 1.24a.

eMSCA note:
A Norwegian Environment Agency screening programme (2019) reports outcomes of a screening program for 85 prioritized main substances. The occurrence of a selection of REACH substances, persistent, mobile, and toxic (PMT) substances from JPI Water Promote and some additional compounds were targeted in various matrices throughout the environment. Among these substances, the quaternary ammonium compounds were also monitored.

The objective of the project was to screen the presence and potential sources of these substances in the Norwegian marine and freshwater environments, as well as in ambient air.

The data obtained from Norwegian program has no effect on the conclusion for the Risk Assessment for the Substance, but only report available scientific literature indicating the moderate to high presence of the Substance in some matrices (marine water, freshwater sediments, and muds/soil).

7.13. Risk characterisation

In general, eMSCA agrees with the approach taken by the Registrant(s) in performing the exposure and risk assessment for all environment compartments.

Following the assessment, the eMSCA concludes that the new data available, provided by the Registrant(s), are suitable to consider that the risk is adequately controlled for all the environmental compartments, since all the respective RCR values are below 1.

References

Registration dossier for the Substance: European Chemicals Agency https://echa.europa.eu/home

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7.14. Abbreviations

ATAC: alkyltrimethylammonium

BAC: alkyldimethylbenzyl

BCF: Bioconcentration factor

CAS: Chemical abstracts service

C&L: Classification and labelling

CLP: Classification, labelling and packaging (Regulation (EC) No 1272/2008)

CMC: Critical Micelle Concentration

CSA: Chemical Safety Assessment

CSR: Chemical Safety Report

DDAC: dialkyldimethylammonium

DOC: Dissolved Organic Carbon (analysis)

DHTDMAC: di(hydrogenated tallow alkyl)dimethylammonium chloride

DODMAC: dimethyldioctadecylammonium chloride

DMEL: Derived Minimal Effect Level

DNEL: Derived no effect level

EC10: the effect concentration at which 10% effect (mortality, inhibition of growth, reproduction, etc) is observed compared to the control group

EC50: the effect concentration at which 10% effect (mortality, inhibition of growth, reproduction, etc) is observed compared to the control group

eMSCA: Evaluating Member State Competent Authority

EPM: Equilibrium Partitioning Method

ERC: Environmental Release Category

ErC50: the concentration of test substance which results in a 50 percent reduction in growth rate relative to the control within 72hrs exposure.

ErC10: the concentration of test substance which results in a 10 percent reduction in growth rate relative to the control within 72hrs exposure.

HPLC: High Performance Liquid Chromatography

KNN: K-Nearest Neighbours

LC50: Lethal Concentration 50

NOEC: No Observed Effect Concentration

NMR: Nuclear Magnetic Resonance

OECD: Organisation for Economic Co-operation and Development

PBT: Persistent Bioaccumulative Toxic

PEC: Predicted Environmental Concentration

PMT: Persistent Mobile Toxic

PNEC: Predicted No-Effect Concentration

QACs: (or quats) Quaternary Ammonium Compounds

QSAR: Quantitative Structure-Activity Relationship

QPRFs: QSAR Prediction Reporting Format

RCR: Risk Characterization Ratio

SEV: Substance Evaluation

SPERC-ECMA: Specific Environmental Release Categories - European Computer Manufacturers Association

STP: Sewage Treatment Plant

UVCB: Unknown or Variable Composition, complex reaction products or Biological materials

vPvB: very Persistent and very Bioaccumulative

WSF: Water Soluble Fractions