Justification Document for the Selection of a CoRAP Substance

Substance Name (public name):	Trimethyloctadecylammonium chloride
EC Number:	203-929-1
CAS Number:	112-03-8
Authority:	Italian CA
Date:	20/03/2018

Cover Note

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

1 IDENTITY OF THE SUBSTANCE

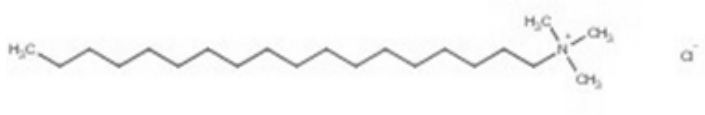
1.1 Other identifiers of the substance

Table: Other Substance identifiers

EC name (public):	Trimethyloctadecylammonium chloride
IUPAC name (public):	N,N,N-trimethyloctadecan-1-aminium chloride
Index number in Annex VI of the CLP Regulation:	-
Molecular formula:	C21H46N.Cl
Molecular weight or molecular weight range:	348.05
Synonyms:	C18 TMAC 1-Octadecanaminium, N,N,N-trimethyl-, chloride

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

Structural formula:



Other relevant information about substance composition

Confidential information.

1.2 Similar substances/grouping possibilities

Has read-across been used by the registrant for the concern related endpoints? ☒ Yes ☐ No

Is the substance a member of a category? ☒ Yes ☐ No

The substance is a member of the Quaternary ammonium salts (QAS) category.

Quaternary ammonium salts (QAS) are salts of a quaternary ammonium cation combined with a negatively charged anion. The category includes alkyltrimethyl QAS (TMAC), benzyl alkyldimethyl QAS (ADBAC) and alkyl ethyl dimethyl ethyl sulphate QAS (ADMAES).

Nine substances have been identified and considered within this QAS category:

TMAC

- Quaternary ammonium compounds, C12-C18 (even numbered) alkyltrimethyl chloride (R=C12-18)

- Cetrimonium chloride (R=C16)

- Quaternary ammonium compounds, (hydrogenated tallow alkyl)trimethyl, chlorides (R=C16-18)

- Quaternary ammonium compounds, (C16-18 and C18-unsatd. alkyl)trimethyl, chlorides (R=C16-18 and C18-unsatd.)

- Trimethyloctadecylammonium chloride (R=C18)

ADBAC

- Quaternary ammonium compounds, benzyl-C12-C16 (even numbered)-alkyldimethyl, chlorides (R=C12-16)

- Quaternary ammonium compounds, benzyl-C12-14 (even numbered)-alkyldimethyl, chlorides (R=C12-14)

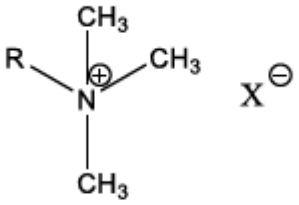
- Quaternary ammonium compounds, benzyl-C16-C18 (even numbered)-alkyldimethyl, chlorides (R=C16-18)

ADMAES

- Quaternary ammonium compounds, C12-14 (even-numbered)-alkylethyldimethyl, ethyl sulphates (R=C12-14)

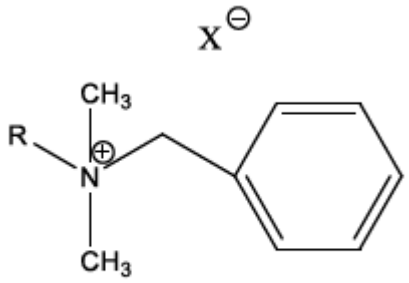
Structural formula:

Representative structure of quaternary ammonium compounds, alkyltrimethyl ammonium chloride (TMAC)



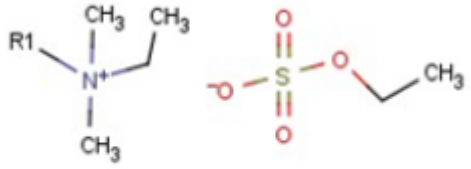
X= Cl^-; R=C12-18

Representative structure of quaternary ammonium compounds, benzyl alkyldimethyl ammonium chloride (ADBAC)



X= Cl^-; R=C12-18

Representative structure of quaternary ammonium compounds, alkyl ethyl dimethyl ethyl sulphate (ADMAES)



R=C12-18

2 OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

No other completed or ongoing processes

Table: Completed or ongoing processes

RMOA	☐ Risk Management Option Analysis (RMOA)	
REACH Processes	Evaluation	☐ Compliance check, Final decision
		☐ Testing proposal, Final decison
		☐ CoRAP and Substance Evaluation
	Authorisation	☐ Candidate List
		☐ Annex XIV

	Restri -ction	☐ Annex XVII[1]
Harmonised C&L		☐ Annex VI (CLP) (see section 3.1)
Processes under other EU legislation		☐ Plant Protection Products Regulation Regulation (EC) No 1107/2009
		☐ Biocidal Product Regulation Regulation (EU) 528/2012 and amendments
Previous legislation		☐ Dangerous substances Directive Directive 67/548/EEC (NONS)
		☐ Existing Substances Regulation Regulation 793/93/EEC (RAR/RRS)
(UNEP) Stockholm convention (POPs Protocol)		☐ Assessment
		☐ In relevant Annex
Other processes / EU legislation		☐ Other (provide further details below)

3 HAZARD INFORMATION (INCLUDING CLASSIFICATION)

3.1 Classification

3.1.1 Harmonised Classification in Annex VI of the CLP

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

[1] Please specify the relevant entry.

3.1.2 Self classification

- In the registration:

Acute Tox. 4	H302
Acute Tox. 3	H311
Skin Corr. 1C	H314
Eye Dam. 1	H318
Aquatic Acute 1	H400 (M-Factor = 10)
Aquatic Chronic 1	H410 (M-Factor = 1)

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

Acute Tox. 4	H312
Skin Corr. 1B	H314
Not Classified	
Skin Irrit. 2	H315
Eye Irrit. 2	H319
Acute Tox. 4	H332
STOT SE 3	H335

4 INFORMATION ON (AGGREGATED) TONNAGE AND USES[2]

4.1 Tonnage and registration status

Table: Tonnage and registration status

From ECHA dissemination site (12/05/17)		
☒ Full registration(s) (Art. 10)	☐ Intermediate registration(s) (Art. 17 and/or 18)	
Tonnage band (as per dissemination site)		
☐ 1 – 10 tpa	☐ 10 – 100 tpa	☒ 100 – 1000 tpa
☐ 1000 – 10,000 tpa	☐ 10,000 – 100,000 tpa	☐ 100,000 – 1,000,000 tpa
☐ 1,000,000 – 10,000,000 tpa	☐ 10,000,000 – 100,000,000 tpa	☐ > 100,000,000 tpa
☐ <1 . . . . . >+ tpa (e.g. 10+ ; 100+ ; 10,000+ tpa)		☐ Confidential
This substance has 1 active registration under REACH, 1 Joint Submission and 0 Individual Submission.		

4.2 Overview of uses

Table: Uses

Part 1:

☒ Manufacture	☒ Formulation	☐ Industrial use	☒ Professional use	☒ Consumer use	☐ Article service life	☐ Closed system

Part 2:

	Use(s)
Uses as intermediate	
Formulation	This substance is used in the following products: cosmetics and personal care products. Release to the environment of this substance is likely to occur from industrial use: formulation of mixtures.

[2] *Please provide here the date when the dissemination site was accessed.*

Uses at industrial sites	
Uses by professional workers	This substance is used in the following products: washing & cleaning products. Other release to the environment of this substance is likely to occur from: indoor use as processing aid.
Consumer Uses	This substance is used in the following products: air care products, washing & cleaning products and cosmetics and personal care products. Other release to the environment of this substance is likely to occur from: indoor use as processing aid.
Article service life	

Part 3: There is high potential for exposure of

☒ Humans	☒ Environment

5. JUSTIFICATION FOR THE SELECTION OF THE CANDIDATE CoRAP SUBSTANCE

5.1. Legal basis for the proposal

☒ Article 44(2) (refined prioritisation criteria for substance evaluation)

☐ Article 45(5) (Member State priority)

5.2. Selection criteria met (why the substance qualifies for being in CoRAP)

☐ Fulfils criteria as CMR/ Suspected CMR

☐ Fulfils criteria as Sensitiser/ Suspected sensitiser

☐ Fulfils criteria as potential endocrine disrupter

☒ Fulfils criteria as PBT/vPvB / Suspected PBT/vPvB

☐ Fulfils criteria high (aggregated) tonnage (*tpa > 1000*)

☒ Fulfils exposure criteria

☒ Fulfils MS's (national) priorities

5.3. Initial grounds for concern to be clarified under Substance Evaluation

Hazard based concerns		
CMR ☐ C ☐ M ☐ R	Suspected CMR[1] ☐ C ☐ M ☐ R	☐ Potential endocrine disruptor
☐ Sensitiser	☐ Suspected Sensitiser[3]	
☐ PBT/vPvB	☒ Suspected PBT/vPvB[1]	☐ Other (please specify below)

Exposure/risk based concerns		
☒ Wide dispersive use	☐ Consumer use	☐ Exposure of sensitive populations
☒ Exposure of environment	☐ Exposure of workers	☐ Cumulative exposure
☐ High RCR	☐ High (aggregated) tonnage	☐ Other (please specify below)

PBT ASSESSMENT

PERSISTENCE

A reliable screening test for biodegradation in water, following the OECD Guideline 301D, showed that the substance was not readily biodegradable: 18% degradation after 28 days. Two additional enhanced screening tests, according to the OECD Guideline 301D, were provided. The criteria for ready biodegradability, within the extended duration of 60d, were not fulfilled (in one test there was 53% degradation after 35d and in the other test was: 77% after 175d; 30% after 30d; 57% after 84d). The Registrants based the conclusion of the assessment as not P, on the results of these two latter studies, considering the substance as inherently biodegradable.
In conclusion, based on the screening information, the substance is potentially P or vP.
A simulation test on biodegradation in soil with the read-across substance quaternary ammonium compounds, benzyl-C12-C16 (even numbered)-alkyldimethyl chlorides (C12-16 ADBAC), EC 939-253-5, was provided. A half-life in soil of 40d was showed, however, the study followed non-standard guideline and the study summary was poorly reported. Information on the source and the density of the inoculums were missing, as well as on any pre-treatment of the inoculums. Therefore the study couldn't be sufficiently validate, consequently a gap in standard REACH information requirements was identified.

BIOACCUMULATION

Two reliable aquatic bioaccumulation studies showed that the substance is not bioaccumulative. The BCF value used for the CSA is = 70.8 L/kg obtained from the QSAR estimation (BCFBAF v3.01

[3] CMR/Sensitiser: known carcinogenic and/or mutagenic and/or reprotoxic properties/known sensitising properties (according to CLP harmonized or registrant self-classification or CLP Inventory)
Suspected CMR/Suspected sensitiser: suspected carcinogenic and/or mutagenic and/or reprotoxic properties/suspected sensitising properties (not classified according to CLP harmonized or registrant self-classification)
Suspected PBT: Potentially Persistent, Bioaccumulative and Toxic

program of EPIWEB v 4.1). Moreover the partition coefficient n-ocotanol/water determined using an estimation method was 3.61 at 25°C.

On the other hand, the substance showed an estimated partition coefficient n-octanol/air equal to log Koa = 11.29 (KOAWIN v3.01 program of EPIWEB v 4.1), that is above the threshold of 5, indicating a potential to bioaccumulate in terrestrial organisms. In addition, one of the constituent, cetrimonium chloride (1-Hexadecanaminium, N,N,N-trimethyl-, chloride, EC 203-928-6, 3 % (w/w), concentration range: >=0 - <=5 % (w/w)), showed an estimated log Koa = 11.15 (Log Kow = 3.23). Other considerations in support of a potential terrestrial bioaccumulation are: the high Log Koc of 5.5 – 6.4 and the tendency to distribute to soil (45.8%) and sediments (48.8%). Moreover the substance showed some evidence of uptake in mammals based on Acute Tox 3/4 self-classification and to accumulate in fatty tissues because of the high octanol solubility (200000 mg/L).

Therefore, although aquatic bioaccumulation potential could be excluded, despite the log Kow is just above the lower limit, a potential to bioaccumulate in terrestrial organisms cannot be excluded.

TOXICITY

Based on the aquatic toxicity data, the lowest long-term toxicity result was a NOEC value of 0.0068 mg a.i./L, obtained with Daphnia magna, for the read-across substance, quaternary ammonium compounds, trimethyltallow alkyl, chlorides (C16-18 and C18-unsatd. TMAC), according to OECD Guideline 211. This value is lower than the 0.01 mg/L limit in a PBT assessment, therefore the substance is toxic (T).

EXPOSURE ASSESSMENT

Trimethyloctadecylammonium chloride is used by consumers and by professional workers (widespread uses) in the following products: air care products, washing & cleaning products and cosmetics and personal care products. The potential for releases to the environment is likely to occur from: indoor use as processing aid.

Moreover, a potential release to the environment of this substance is likely to occur from industrial use: formulation of mixtures.

RISK CONSIDERATIONS

The substance pose a concern as suspected PBT, that need to be further examined and clarified under SEV. The substance has wide dispersive uses, therefore a potential risk for human health and for the environment is expected. The requested information under CoRAP process would lead to improvement of Risk management Measures for the substance.

5.4. Preliminary indication of information that may need to be requested to clarify the concern

☐ Information on toxicological properties	☐ Information on physico-chemical properties
☒ Information on fate and behaviour	☐ Information on exposure
☐ Information on ecotoxicological properties	☐ Information on uses

☐ Information on ED potential	☐ Other (provide further details below)
Definitive studies on biodegradability are required to conclude on the P property of the substance (simulation test in surface water, OECD TG 309), that are standard REACH information requirements. Depending on the output of the P assessment, the B criterion can then be considered. An experimental study on terrestrial bioaccumulation (OECD TG 317: Bioaccumulation in Terrestrial Oligochaetes) could be necessary for a proper evaluation.	

5.5. Potential follow-up and link to risk management

☐ Harmonised C&L	☐ Restriction	☐ Authorisation	☒ Other (provide further details)
In case a PBT concern was confirmed, because the dossiers suggest that the uses are wide dispersive, a risk management option analysis (RMOA) could be necessary to decide on a potential regulatory RMO.			