



Justification Document for the Selection of a CoRAP Substance

| | |
|--------------------------------------|--|
| Substance Name (public name): | Betaines, C12-14 (even numbered)-alkyldimethyl |
| EC Number: | 931-700-2 |
| CAS Number: | - |
| Authority: | France |
| Date: | 21/03/2017 |

Cover Note

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

| | | |
|-----------|--|-----------|
| 1 | IDENTITY OF THE SUBSTANCE | 3 |
| 1.1 | Other identifiers of the substance | 3 |
| 2 | OVERVIEW OF OTHER PROCESSES / EU LEGISLATION | 9 |
| 3 | HAZARD INFORMATION (INCLUDING CLASSIFICATION) | 11 |
| 3.1 | Classification | 11 |
| 3.1.1 | Harmonised Classification in Annex VI of the CLP | 11 |
| 3.1.2 | Self classification | 11 |
| 3.1.3 | Proposal for Harmonised Classification in Annex VI of the CLP | 11 |
| 4 | INFORMATION ON (AGGREGATED) TONNAGE AND USES | 12 |
| 4.1 | Tonnage and registration status | 12 |
| 4.2 | Overview of uses | 12 |
| 5. | JUSTIFICATION FOR THE SELECTION OF THE CANDIDATE CORAP SUBSTANCE | 14 |
| 5.1. | Legal basis for the proposal | 14 |
| 5.2. | Selection criteria met (why the substance qualifies for being in CoRAP) | 14 |
| 5.3 | Initial grounds for concern to be clarified under Substance Evaluation | 14 |
| 5.4 | Preliminary indication of information that may need to be requested to clarify the concern | 15 |
| 5.5 | Potential follow-up and link to risk management | 16 |

1 IDENTITY OF THE SUBSTANCE

1.1 Other identifiers of the substance

Table: Other Substance identifiers

| | |
|--|--|
| EC name (public): | Betaines, C12-14 (even numbered)-alkyldimethyl |
| IUPAC name (public): | Betaines, C12-14 (even numbered)-alkyldimethyl |
| Index number in Annex VI of the CLP Regulation: | |
| Molecular formula: | C16H33NO2 C18H37NO2 |
| Molecular weight or molecular weight range: | >= 271.0 - <=299.49 |
| Synonyms: | Alkyl Dimethyl Betaine Betaines, C12-14 (even numbered)-alkyldimethyl |

Type of substance Mono-constituent Multi-constituent UVCB

Structural formula:

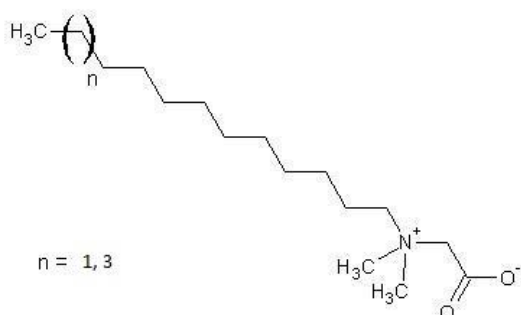


Table: Constituent

| | |
|--|--|
| EC number: | 931-700-2 |
| EC name (public): | Betaines, C12-14 (even numbered)-alkyldimethyl |
| CAS number: | - |
| CAS name (public): | - |
| IUPAC name (public): | Alkyl Dimethyl Betaine Betaines, C12-14 (even numbered)-alkyldimethyl |
| Index number in Annex VI of the CLP Regulation: | |
| Molecular formula: | C16H33NO2 C18H37NO2 |
| Molecular weight or molecular weight range: | >= 271.0 - <=299.49 |
| Synonyms: | Alkyl Dimethyl Betaine Betaines, C12-14 (even numbered)-alkyldimethyl |

Table: Constituent

| | |
|--|---|
| EC number: | 231-598-3 |
| EC name (public): | Sodium chloride |
| CAS number: | 7647-14-5 |
| CAS name (public): | |
| IUPAC name (public): | sodium chloride |
| Index number in Annex VI of the CLP Regulation: | |
| Molecular formula: | CINa |
| Molecular weight or molecular weight range: | 58.443 |
| Synonyms: | NaCl Reaction mass of sodium and chlorine Sirsal Sodium Chloride Sodium Chloride, USP |

There is a self-classification of substance CAS #7647-14-5 as Eye irrit. 2, skin irrit. 2, skin mild Irrit. 3 and STOT RE 2.

Table: Constituent

| | |
|--|--|
| EC number: | 220-624-9 |
| EC name (public): | Sodium glycollate |
| CAS number: | 2836-32-0 |
| CAS name (public): | |
| IUPAC name (public): | Sodium glycollate |
| Index number in Annex VI of the CLP Regulation: | |
| Molecular formula: | C ₂ H ₃ O ₃ .Na |
| Molecular weight or molecular weight range: | 98.033 |
| Synonyms: | Acetic acid, hydroxy-, monosodium salt |

There is a self-classification of substance CAS #2836-32-0 as Eye irrit. 2, skin irrit. 2, and STOT SE 3.

Table: Constituent

| | |
|--|--|
| EC number: | 211-748-4 |
| EC name (public): | (carboxylatomethyl)hexadecyldimethylammonium |
| CAS number: | 693-33-4 |
| CAS name (public): | |
| IUPAC name (public): | Betaines, C16-Alkyldimethyl |
| Index number in Annex VI of the CLP Regulation: | |
| Molecular formula: | C ₂₀ H ₄₁ NO ₂ |
| Molecular weight or molecular weight range: | 327.549 |
| Synonyms: | (Carboxylatomethyl)hexadecyldimethylammonium 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, inner salt 14151_693-33-4 Cetyl dimethyl betaine [hexadecyl(dimethyl)ammonio]acetate |

There is a self-classification of substance CAS #693-33-4 as Skin Irrit. 2, Eye irrit. 2 and acute tox. 4.

Table: Constituent

| | |
|--|------------------------------|
| EC number: | 238-464-9 |
| EC name (public): | Amines, C12-14-alkyldimethyl |
| CAS number: | 84649-84-3 |
| CAS name (public): | |
| IUPAC name (public): | Amines, C12-14-Alkyldimethyl |
| Index number in Annex VI of the CLP Regulation: | |
| Molecular formula: | C14H31N C16H35N |
| Molecular weight or molecular weight range: | 213 - 241 |
| Synonyms: | |

There is a self-classification of substance CAS #84649-84-3 as acute tox. 4, skin corr. 1B, Aquatic acute 1 and aquatic chronic 1.

1.2 Similar substances/grouping possibilities

| Chemical name | Betaines, C12-14 (even numbered)-alkyldimethyl | Betaines, C12-14 (even numbered)-alkyldimethyl | Betaines, coco alkyldimethyl (C8-18) | Dodecyl dimethyl betaine | Tetradecyl dimethyl betaine |
|---------------|--|--|--------------------------------------|--------------------------|-----------------------------|
| | Target chemical | grouping possibilities | | | |
| CAS no | - | 66455-29-6 | 68424-94-2 | 683-10-3 | 2601-33-4 |
| EC no | 931-700-2 | 266-368-1 | 270-329-4 | 211-669-5 | 220-006-9 |

Table: Constituent

| | |
|--|---|
| EC number: | 266-368-1 |
| EC name (public): | Betaines, C12-14-alkyldimethyl |
| CAS number: | 66455-29-6 |
| CAS name (public): | |
| IUPAC name (public): | |
| Index number in Annex VI of the CLP Regulation: | |
| Molecular formula: | |
| Molecular weight or molecular weight range: | |
| Synonyms: | (C12-14) Alkyl dimethyl betaine - 13961_66455-29-6 Alkyldimethyl betaine Betaines, C12-14-alkyldimethyl |

Structural formula: -

There is a self-classification of substance CAS #66455-29-6 as skin irrit. 2, skin corr. 1B, Eye dam. 1, Eye irrit. 2, STOT SE3, aquatic chronic 3 and aquatic acute 1.

Table: Constituent

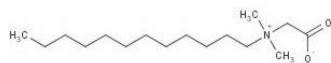
| | |
|--|---|
| EC number: | 270-329-4 |
| EC name (public): | Betaines, coco alkyldimethyl (C8-18) |
| CAS number: | 68424-94-2 |
| CAS name (public): | |
| IUPAC name (public): | Betaines, Coco alkyldimethyl Betains, coco alkyldimethyl |
| Index number in Annex VI of the CLP Regulation: | |
| Molecular formula: | |
| Molecular weight or molecular weight range: | |
| Synonyms: | |

Structural formula: -

There is a self-classification of substance CAS #68424-94-2 as skin irrit. 2, skin corr. 1B, skin sens. 1A, Eye dam. 1, Eye irrit. 2, aquatic chronic 3 and aquatic acute 1.

Table: Constituent

| | |
|--|---|
| EC number: | 211-669-5 |
| EC name (public): | (carboxylatomethyl) dodecyldimethylammonium |
| CAS number: | 683-10-3 |
| CAS name (public): | |
| IUPAC name (public): | (carboxylatomethyl)dodecyldimethylammonium (Lauryldimethylammonio)acetate 1-dodecanaminium, n-(carboxymethyl)-n,n-dimethyl-, inner salt 2-(dodecyldimethylazaniumyl)acetate carboxylatomethyl)dodecyldimethylammonium sodium 2-[dodecyl(dimethyl)azaniumyl]acetate chloride [docecyldimethylammonio]acetate [dodecyl(dimethyl)ammonio]acetate |
| Index number in Annex VI of the CLP Regulation: | |
| Molecular formula: | C ₁₆ H ₃₃ N ₂ O ₂ |
| Molecular weight or molecular weight range: | |
| Synonyms: | |

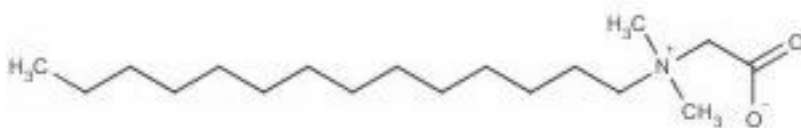
Structural formula:

There is a self-classification of substance CAS #683-10-3 as skin irrit. 2, acute tox. 3 and 4, skin corr. 1B, skin sens. 1, Eye dam. 1, STOT SE 2, aquatic chronic 3 and aquatic acute 1.

Table: Constituent

| | |
|--|---|
| EC number: | 220-006-9 |
| EC name (public): | (carboxylatomethyl)dimethyltetradecylammonium |
| CAS number: | 2601-33-4 |
| CAS name (public): | |
| IUPAC name (public): | (Carboxylatomethyl)dimethyltetradecylammonium [dimethyl(tetradecyl)ammonio]acetate |
| Index number in Annex VI of the CLP Regulation: | - |
| Molecular formula: | C ₁₈ H ₃₇ NO ₂ |
| Molecular weight or molecular weight range: | |
| Synonyms: | (Carboxylatomethyl)dimethyltetradecylammonium [dimethyl(tetradecyl)ammonio]acetate |

Structural formula:



There is a self-classification of substance CAS #2601-33-4 as skin irrit. 2, skin sens. 1, skin corr. 1B, Eye dam. 1, STOT SE3 and aquatic chronic 3.

2 OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

Table: Completed or ongoing processes

| | | |
|---------------|---|--|
| RMOA | <input type="checkbox"/> Risk Management Option Analysis (RMOA) | |
| | REACH Processes | Evaluation |
| Evaluation | | <input checked="" type="checkbox"/> Testing proposal, Final decision |
| Evaluation | | <input type="checkbox"/> CoRAP and Substance Evaluation |
| Authorisation | | <input type="checkbox"/> Candidate List |
| Authorisation | <input type="checkbox"/> Annex XIV | |

JUSTIFICATION DOCUMENT FOR THE SELECTION OF A CORAP SUBSTANCE

| | | |
|---|-------------------|---|
| | Restri- -ction | <input type="checkbox"/> Annex XVII |
| Harmonised C&L | | <input type="checkbox"/> Annex VI (CLP) (see section 3.1) |
| Processes under other EU legislation | | <input type="checkbox"/> Plant Protection Products Regulation Regulation (EC) No 1107/2009 |
| | | <input type="checkbox"/> Biocidal Product Regulation Regulation (EU) 528/2012 and amendments |
| Previous legislation | | <input type="checkbox"/> Dangerous substances Directive Directive 67/548/EEC (NONS) |
| | | <input type="checkbox"/> Existing Substances Regulation Regulation 793/93/EEC (RAR/RRS) |
| (UNEP) Stockholm convention (POPs Protocol) | | <input type="checkbox"/> Assessment |
| | | <input type="checkbox"/> In relevant Annex |
| Other processes / EU legislation | | <input checked="" type="checkbox"/> Other (provide further details below) |
| As a surfactant, some of the substance uses are submitted to the detergent legislation (EC/648/2004). | | |

3 HAZARD INFORMATION (INCLUDING CLASSIFICATION)

3.1 Classification

3.1.1 Harmonised Classification in Annex VI of the CLP

No harmonised classification.

3.1.2 Self classification

- In the registration dossier:
 - Skin Corr. 1B, H314
 - Eye Dam. 1, H318
 - Aquatic Chronic 3, H412
- The following hazard classes are in addition notified among the aggregated self classifications in the C&L Inventory:

| Classification | | |
|-----------------------------------|--------------------------|--------------------------|
| Hazard Class and Category Code(s) | Hazard Statement Code(s) | Hazard Statement Code(s) |
| Skin Corr. 1B | H314 | H314 |
| Eye Dam. 1 | H318 | |
| Aquatic Chronic 3 | H412 | H412 |
| Skin Corr. 1B | H314 | H314 |
| Eye Dam. 1 | H318 | |
| Aquatic Chronic 3 | H412 | H412 |
| Skin Irrit. 2 | H315 | H315 |
| Eye Dam. 1 | H318 | H318 |
| Skin Corr. 1B | H314 | H314 |
| Eye Dam. 1 | H318 | |

3.1.3 Proposal for Harmonised Classification in Annex VI of the CLP

Not applicable

4 INFORMATION ON (AGGREGATED) TONNAGE AND USES¹

4.1 Tonnage and registration status

Table: Tonnage and registration status

| | | |
|--|---|--|
| From ECHA dissemination site | | |
| <input checked="" type="checkbox"/> Full registration(s) (Art. 10) | <input type="checkbox"/> Intermediate registration(s) (Art. 17 and/or 18) | |
| Tonnage band (as per dissemination site) | | |
| <input type="checkbox"/> 1 - 10 tpa | <input type="checkbox"/> 10 - 100 tpa | <input type="checkbox"/> 100 - 1000 tpa |
| <input checked="" type="checkbox"/> 1000 - 10,000 tpa | <input type="checkbox"/> 10,000 - 100,000 tpa | <input type="checkbox"/> 100,000 - 1,000,000 tpa |
| <input type="checkbox"/> 1,000,000 - 10,000,000 tpa | <input type="checkbox"/> 10,000,000 - 100,000,000 tpa | <input type="checkbox"/> > 100,000,000 tpa |
| <input type="checkbox"/> <1 >+ tpa (e.g. 10+ ; 100+ ; 10,000+ tpa) | | <input type="checkbox"/> Confidential |
| Joint submission | | |

4.2 Overview of uses

This substance is used in the following products: washing & cleaning products, metal surface treatment products, textile treatment products and dyes and polishes and waxes.

This substance is used in the following areas: formulation of mixtures and/or re-packaging. This substance is used for the manufacture of: textile, leather or fur.

This substance can be found in products with material based on: fabrics, textiles and apparel (e.g. clothing, mattress, curtains or carpets, textile toys) and plastic (e.g. food packaging and storage, toys, mobile phones). This substance is intended to be released from scented: clothes.

Table: Uses

Part 1:

| | | | | | | |
|---|---|--|--|--|--|--|
| <input checked="" type="checkbox"/> Manufacture | <input checked="" type="checkbox"/> Formulation | <input checked="" type="checkbox"/> Industrial use | <input checked="" type="checkbox"/> Professional use | <input checked="" type="checkbox"/> Consumer use | <input checked="" type="checkbox"/> Article service life | <input type="checkbox"/> Closed system |
|---|---|--|--|--|--|--|

Part 2:

| | |
|-----------------------------|---------------|
| | Use(s) |
| Uses as intermediate | |

¹ Dissemination site was accessed in April 2016.

JUSTIFICATION DOCUMENT FOR THE SELECTION OF A CORAP SUBSTANCE

| | |
|-------------------------------------|--|
| Formulation | Cosmetics, personal care products |
| Uses at industrial sites | Cleaning and maintenance products (i.e. degreaser, lubricant) Metal treatment products, including galvanic and electroplating products Processing aids for textile, leather production Surface treatment (coating) Cosmetic, washing and cleaning products formulation Laboratory chemicals |
| Uses by professional workers | washing and cleaning products (including solvent based products) Laboratory chemicals cosmetics, personal care products |
| Consumer Uses | Polishes and wax blends Biocidal products (e.g. disinfectants, pest control) Air care products Washing and cleaning products (including solvent based products) Cosmetics, personal care products |
| Article service life | Textile article Plastic |

Part 3: There is high potential for exposure of

| | |
|--|---|
| <input checked="" type="checkbox"/> Humans | <input checked="" type="checkbox"/> 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 <input type="checkbox"/> C <input type="checkbox"/> M <input type="checkbox"/> R | Suspected CMR ¹ <input type="checkbox"/> C <input type="checkbox"/> M <input checked="" type="checkbox"/> R | <input type="checkbox"/> Potential endocrine disruptor |
| <input type="checkbox"/> Sensitiser | <input type="checkbox"/> Suspected Sensitiser ² | |
| <input type="checkbox"/> PBT/vPvB | <input type="checkbox"/> Suspected PBT/vPvB ¹ | <input checked="" type="checkbox"/> Other (please specify below) |
| Exposure/risk based concerns | | |
| <input checked="" type="checkbox"/> Wide dispersive use | <input checked="" type="checkbox"/> Consumer use | <input type="checkbox"/> Exposure of sensitive populations |
| <input checked="" type="checkbox"/> Exposure of environment | <input checked="" type="checkbox"/> Exposure of workers | <input type="checkbox"/> Cumulative exposure |
| <input checked="" type="checkbox"/> High RCR | <input checked="" type="checkbox"/> High (aggregated) tonnage | <input type="checkbox"/> Other (please specify below) |

² 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

The lead registrant considers that inhalation studies are not required because the test substance has a low vapour pressure, exposure to aerosols, particles or droplets is unlikely. However uses as sprays cannot be excluded and inhalation route has to be considered in the CSA.

Furthermore there is a data gap for repeated-dose study by inhalation route as an inhalation exposure is very likely to occur due to the use of substance. A prior CCH would confirm the identified concern.

Reproductive toxicity studies showed several developmental toxicity effects like reduced pup weight, litter size and increased post-implantation and postnatal loss. The registrant considers that these effects have to be considered as secondary to maternal toxicity. However additional information are necessary to confirm this statement and a concern for developmental toxicity remains. A prior CCH would confirm the identified concern.

For the human risk assessment, the preliminary analysis of the dossier revealed high RCRs for some applied scenarios like professional surface cleaning, industrial cleaning or spraying. Furthermore, the model used may underestimate exposure due to the vapor pressure of the substance and the formation of aerosol e.g. for spraying use. Considering the widespread uses and some flaws in the exposure assessment, the human risk assessment should be analysed further, in order to confirm that all assessed uses are safe for workers and consumers.

For the environmental risk assessment, the preliminary analysis of the dossier revealed high RCRs for some applied scenarios like industrial cleaning for soil and sediment. Considering the widespread uses, including wide dispersive uses, the high tonnage, the environmental risk assessment should be analysed further, in order to confirm that all assessed uses are safe for the environment.

Additionally concerning e-fate and behavior since the QSAR predictions for e-fate and behavior included in the registration dossier are not considered as reliable therefore additional data may be needed for these endpoints. And the data available for aquatic toxicity will need to be carefully assessed.

Several read-across are proposed in the registration dossiers which may be relevant, nevertheless the relevance of these read-across will be further evaluate during the evaluation phase and will conclude if this read-across is acceptable.

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

the concern

| | |
|--|---|
| <input checked="" type="checkbox"/> Information on toxicological properties | <input type="checkbox"/> Information on physico-chemical properties |
| <input checked="" type="checkbox"/> Information on fate and behaviour | <input checked="" type="checkbox"/> Information on exposure |
| <input checked="" type="checkbox"/> Information on ecotoxicological properties | <input checked="" type="checkbox"/> Information on uses |
| <input type="checkbox"/> Information on ED potential | <input type="checkbox"/> Other (provide further details below) |

Deeper analysis of the existing data (existing or to be generated following CCH) need to be performed before identifying the information that might be necessary to ensure safe use of the chemical.

Additionally concerning e-fate and behavior, the QSAR predictions for e-fate and behavior are not considered as reliable therefore additional data may be needed for these endpoints.

5.5 Potential follow-up and link to risk management

| | | | |
|--|---|--|--|
| <input checked="" type="checkbox"/> Harmonised C&L | <input checked="" type="checkbox"/> Restriction | <input type="checkbox"/> Authorisation | <input type="checkbox"/> Other (provide further details) |
| <p>Doubts are linked to endpoints that could warrant a CLH. On the other hand, uses have been identified with high exposure compared to existing limit values (PNECs and DNELs) that might warrant restrictions of certain uses.</p> | | | |