

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 17.06.2014

Version 8.9

SECTION 1. Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Catalogue No. 814858

Product name Alkylbenzyltrimethylammonium chloride (50% solution in water) for synthesis

REACH Registration Number This product is a mixture. REACH Registration Number see section 3.

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses Chemical for synthesis

For additional information on uses please refer to the Merck Chemicals portal (www.merck-chemicals.com).

1.3 Details of the supplier of the safety data sheet

Company Merck KGaA * 64271 Darmstadt * Germany * Phone: +49 6151 72-0

Responsible Department LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number

Please contact the regional company representation in your country.

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Acute toxicity, Category 4, Oral, H302

Skin corrosion, Category 1B, H314

Acute aquatic toxicity, Category 1, H400

For the full text of the H-Statements mentioned in this Section, see Section 16.

Classification (67/548/EEC or 1999/45/EC)

| | | |
|----|-------------------------------|--------|
| C | Corrosive | R34 |
| Xn | Harmful | R21/22 |
| N | Dangerous for the environment | R50 |

For the full text of the R-phrases mentioned in this Section, see Section 16.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H302 Harmful if swallowed.

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H314 Causes severe skin burns and eye damage.
H400 Very toxic to aquatic life.

Precautionary statements

Prevention

P273 Avoid release to the environment.

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H314 Causes severe skin burns and eye damage.

Precautionary statements

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P308 + P311 IF exposed or concerned: Call a POISON CENTER or doctor/ physician.

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

Chemical nature Aqueous solution of organic compounds.

3.1 Substance

not applicable

3.2 Mixture

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

| CAS-No. | Registration number | Classification |
|---|---------------------|----------------|
| benzyltrimethylalkylammonium chloride (C ₁₂ -C ₁₈) (>= 50 % - <= 100 %) | | |
| 68391-01-5 | *) | |

Acute toxicity, Category 4, H302

Acute toxicity, Category 4, H312

Skin corrosion, Category 1B, H314

Acute aquatic toxicity, Category 1, H400

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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For the full text of the H-Statements mentioned in this Section, see Section 16.

Hazardous components (1999/45/EC)

Chemical Name (Concentration)

CAS-No. Classification

benzyltrimethylalkylammonium chloride (C₁₂-C₁₈) (>= 50 % - <= 100 %)

68391-01-5 Xn, Harmful; R21/22

 C, Corrosive; R34

 N, Dangerous for the environment; R50

For the full text of the R-phrases mentioned in this Section, see Section 16.

SECTION 4. First aid measures

4.1 Description of first aid measures

General advice

First aider needs to protect himself.

After inhalation: fresh air. Call in physician.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Call a physician immediately.

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Risk of perforation! Call a physician immediately. Do not attempt to neutralise.

4.2 Most important symptoms and effects, both acute and delayed

Irritation and corrosion, Cough, Shortness of breath, Diarrhoea, Nausea, Vomiting, Risk of blindness!

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), Foam, Dry powder, Water

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

Fire may cause evolution of:

Hydrogen chloride gas, nitrogen oxides

5.3 Advice for firefighters

Special protective equipment for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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Further information

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Do not breathe vapours, aerosols. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

6.2 Environmental precautions

Do not empty into drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7 and 10).

Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Protected from light.

Recommended storage temperature see product label.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

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Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Tightly fitting safety goggles

Hand protection

full contact:

Glove material: natural latex
Glove thickness: 0,6 mm
Break through time: > 480 min

splash contact:

Glove material: Nitrile rubber
Glove thickness: 0,11 mm
Break through time: > 30 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 706 Lapren® (full contact), KCL 741 Dermatrill® L (splash contact).

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

protective clothing

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not empty into drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

| | |
|-----------------|-----------------------------|
| Form | liquid |
| Colour | colourless |
| Odour | characteristic |
| Odour Threshold | No information available. |
| pH | 5 - 7 at 10 g/l 20 °C |
| Melting point | ca. -5 °C |

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| | |
|--|---|
| Boiling point | No information available. |
| Flash point | 160 - 170 °C |
| Evaporation rate | No information available. |
| Flammability (solid, gas) | No information available. |
| Lower explosion limit | No information available. |
| Upper explosion limit | No information available. |
| Vapour pressure | No information available. |
| Relative vapour density | No information available. |
| Density | 0,978 - 0,988 g/cm ³ at 20 °C |
| Relative density | No information available. |
| Water solubility | at 20 °C soluble |
| Partition coefficient: n-octanol/water | No information available. |
| Auto-ignition temperature | No information available. |
| Decomposition temperature | No information available. |
| Viscosity, dynamic | 100 - 300 mPa.s at 20 °C |
| Explosive properties | Not classified as explosive. |
| Oxidizing properties | none |

9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

Sensitivity to light

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

10.4 Conditions to avoid

Strong heating.

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10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Mixture

Acute oral toxicity

absorption

Symptoms: Nausea, Vomiting, Diarrhoea, If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the oesophagus and the stomach., Risk of aspiration upon vomiting., Aspiration may cause pulmonary oedema and pneumonitis.

Acute inhalation toxicity

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Acute dermal toxicity

absorption

Acute toxicity estimate : > 2.000 mg/kg

Calculation method

Skin irritation

rabbit

Result: Causes burns.

(External MSDS)

Mixture causes burns.

Eye irritation

Mixture causes serious eye damage. Risk of blindness!

Sensitisation

This information is not available.

Germ cell mutagenicity

This information is not available.

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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Components

benzyltrimethylalkylammonium chloride (C₁₂-C₁₈)

Acute oral toxicity

LD50 rat: 650 mg/kg (External MSDS)

Acute dermal toxicity

Acute toxicity estimate : 1.101 mg/kg

Expert judgement

SECTION 12. Ecological information

Mixture

12.1 Toxicity

No information available.

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

No information available.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

Substance(s) in the mixture do(es) not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII, or a PBT/vPvB assessment was not conducted.

12.6 Other adverse effects

Discharge into the environment must be avoided.

Components

benzyltrimethylalkylammonium chloride (C₁₂-C₁₈)

Toxicity to fish

LC50 fish: 0,3 - 6,5 mg/l; 96 h (External MSDS)

Toxicity to algae

IC50 algae: 0,62 - 2,1 mg/l (External MSDS)

Biodegradability

8 %; 28 d

OECD Test Guideline 301D

Not readily biodegradable.

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SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number UN 1760
14.2 Proper shipping name CORROSIVE LIQUID, N.O.S. (BENZALKONIUMCHLORIDE SOLUTION)
14.3 Class 8
14.4 Packing group II
14.5 Environmentally hazardous yes
14.6 Special precautions for user yes
Tunnel restriction code E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number UN 1760
14.2 Proper shipping name CORROSIVE LIQUID, N.O.S. (BENZALKONIUMCHLORIDE SOLUTION)
14.3 Class 8
14.4 Packing group II
14.5 Environmentally hazardous yes
14.6 Special precautions for user no

Sea transport (IMDG)

14.1 UN number UN 1760
14.2 Proper shipping name CORROSIVE LIQUID, N.O.S. (BENZALKONIUMCHLORIDE SOLUTION)
14.3 Class 8
14.4 Packing group II
14.5 Environmentally hazardous yes
14.6 Special precautions for user yes
EmS F-A S-B

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
Not relevant

SECTION 15. Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulations

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| | |
|---|--|
| Major Accident Hazard Legislation | 96/82/EC Dangerous for the environment 9a Quantity 1: 100 t Quantity 2: 200 t |
| Occupational restrictions | Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable. |
| Regulation (EC) No 1005/2009 on substances that deplete the ozone layer | not regulated |
| Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC | not regulated |
| Regulation (EC) No 689/2008 concerning the export and import of dangerous chemicals | not regulated |
| Substances of very high concern (SVHC) | This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w). |
| <i>National legislation</i> | |
| Storage class | 8A |

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

Full text of H-Statements referred to under sections 2 and 3.

| | |
|------|--|
| H302 | Harmful if swallowed. |
| H312 | Harmful in contact with skin. |
| H314 | Causes severe skin burns and eye damage. |
| H400 | Very toxic to aquatic life. |



Full text of R-phrases referred to under sections 2 and 3

| | |
|--------|--|
| R21/22 | Harmful in contact with skin and if swallowed. |
| R34 | Causes burns. |
| R50 | Very toxic to aquatic organisms. |

Training advice

Provide adequate information, instruction and training for operators.

Labelling (67/548/EEC or 1999/45/EC)

| | | |
|-----------|---|-------------------------------|
| Symbol(s) |  C | Corrosive |
| |  N | Dangerous for the environment |

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Product name Alkylbenzyldimethylammonium chloride (50% solution in water) for synthesis

| | | |
|---------------------|-------------------|---|
| <i>R-phrases(s)</i> | 21/22-34-50 | Harmful in contact with skin and if swallowed. Causes burns. Very toxic to aquatic organisms. |
| <i>S-phrases(s)</i> | 26-36/37/39-45-61 | In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Avoid release to the environment. Refer to special instructions/ Safety data sheets. |

Reduced labelling (≤125 ml)

Symbol(s)



C

N

R-phrases(s)

21/22-34

S-phrases(s)

26-36/37/39-45

Corrosive

Dangerous for the environment

Harmful in contact with skin and if swallowed. Causes burns.

In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.