

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 15.08.2013

Version 12.9

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

1.1 Product identifier

Catalogue No. 821944
 Product name Alkylbenzyltrimethylammonium chloride 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
 Acute toxicity, Category 4, Dermal, H312
 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 + H312 Harmful if swallowed or in contact with skin

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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.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

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

P309 + P310 IF exposed or if you feel unwell: 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.

P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

not applicable

3.2 Mixture

Formula $[RN(CH_3)_2CH_2C_6H_5]Cl$

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

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*) 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.

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 (C ₁₂ -C ₁₈) (>= 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.

After skin contact: wash off with plenty of water. Immediately remove contaminated clothing. If available swab with polyethylene glycol 400. Call a physician immediately.

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

After swallowing: make victim drink water (two glasses at most), avoid vomiting (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, 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

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.

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. Avoid inhalation of vapours/aerosols or dusts. 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).

Depending on the state of matter, take up with suitable equipment or with liquid-absorbent material (e.g. Chemisorb®). 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. Dry.

Store at +15°C to +25°C.

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:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 480 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 730 Camatril® -Velours (full contact), KCL 730 Camatril® -Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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 dusts/vapours/aerosols are generated.

Recommended Filter type: Filter A-(P2)

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	pasty
Colour	yellow
Odour	aromatic
Odour Threshold	No information available.
pH	6 - 8 at 10 g/l 20 °C

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Melting point	37 - 41 °C
Boiling point	No information available.
Flash point	No information available.
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.
Relative density	No information available.
Water solubility	at 20 °C soluble
Partition coefficient: n-octanol/water	log Pow: 0,9 - 1,8 (External MSDS) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	> 150 °C
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none
9.2 Other data	
Bulk density	800 kg/m ³

SECTION 10. Stability and reactivity

10.1 Reactivity

See section 10.3

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

10.4 Conditions to avoid

no information available

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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

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the oesophagus and the stomach.

absorption

Acute toxicity estimate: 684,21 mg/kg

Calculation method

Acute inhalation toxicity

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

Acute dermal toxicity

Acute toxicity estimate : 1.158 mg/kg

Calculation method

absorption

Skin irritation

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.

Components

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benzyltrimethylalkylammonium chloride (C₁₂-C₁₈)

Acute oral toxicity
LD50 rat: 650 mg/kg (External MSDS)

Acute dermal toxicity
Acute toxicity estimate : 1.100 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

Partition coefficient: n-octanol/water
log Pow: 0,9 - 1,8
(External MSDS) Bioaccumulation is not expected.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Additional ecological information
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 1759
14.2 Proper shipping name CORROSIVE SOLID, N.O.S.
(ALKYLBENZYLDIMETHYLAMMONIUM CHLORIDE)
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 1759
14.2 Proper shipping name CORROSIVE SOLID, N.O.S.
(ALKYLBENZYLDIMETHYLAMMONIUM CHLORIDE)
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 1759
14.2 Proper shipping name CORROSIVE SOLID, N.O.S.
(ALKYLBENZYLDIMETHYLAMMONIUM CHLORIDE)
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 above the respective regulatory limit (> 0.1 % (w/w) Regulation (EC) No 1907/2006 (REACH), Article 57).

National legislation

Storage class 8 A

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
R-phrase(s) 21/22-34-50 Harmful in contact with skin and if swallowed. Causes burns.
Very toxic to aquatic organisms.
S-phrase(s) 26-36/37/39-45-61 In case of contact with eyes, rinse immediately with plenty of

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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 21/22-34

S-phrases 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.