

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

Catalogue No. 814087
Product name Cetyl trimethylammonium chloride (50% solution in 2propanol/water 3:2) for synthesis

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

Identified uses Chemicals for soaps, detergents, maintenance products
For additional information on uses please refer to the Merck Chemicals portal (www.merck-chemicals.com).

1.2 Details of the supplier of the safety data sheet

Company **Swadesh Life Science**
H-103, Sumel 7, Near Soni ni chali
BRTS, Rakhiyal,
Ahmedabad,Gujarat, India

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Flammable liquid, Category 2, H225
Acute toxicity, Category 4, Oral, H302
Skin corrosion, Category 1B, H314
Specific target organ toxicity - single exposure, Category 3, Central nervous system, H336 Acute aquatic toxicity, Category 1, H400

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

F	Highly flammable	R11
C	Corrosive	R34
Xn	Harmful	R22
N	Dangerous for the environment	R50 R67

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H225 Highly flammable liquid and vapour.

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H336 May cause drowsiness or dizziness.

H400 Very toxic to aquatic life.

Precautionary statements

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

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.

Storage

P403 + P235 Store in a well-ventilated place. Keep cool.

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

2.3 Other hazards None known.

SECTION 3. Composition/information on ingredients

Chemical nature Aqueous propanolic solution.

3.1 Substance
not applicable

3.2 Mixture

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

Chemical Name (Concentration)

CAS-No. Registration number Classification

Hexadecyltrimethylammonium chloride ($\geq 50\%$ - $\leq 100\%$)
112-02-7 *)

Acute toxicity, Category 4, H302

Skin corrosion, Category 1B, H314

Acute aquatic toxicity, Category 1, H400

2-Propanol ($\geq 25\%$ - $< 50\%$)

Flammable liquid, Category 2, H225

Eye irritation, Category 2, H319

Specific target organ toxicity - single exposure, Category 3, H336

Hazardous components (1999/45/EC)

Chemical Name (Concentration)

CAS-No. Classification

Hexadecyltrimethylammonium chloride ($\geq 50\%$ - $\leq 100\%$)

112-02-7 Xn, Harmful; R22

C, Corrosive; R34

N, Dangerous for the environment; R50

2-Propanol ($\geq 25\%$ - $< 50\%$)

67-63-0 F, Highly flammable; R11

Xi, Irritant; R36

R67

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: 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, Drowsiness, drowsiness 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.

Forms explosive mixtures with air at ambient temperatures.

Pay attention to flashback.

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

Fire may cause evolution of:

nitrogen oxides, Hydrogen chloride gas

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.

Further information

Suppress (knock down) gases/vapours/mists with a water spray jet. Cool closed containers exposed to fire with water spray. 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: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

6.2 Environmental precautions

Do not empty into drains. Risk of explosion.

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. Chemisorb®). Dispose of properly. Clean up affected area.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Observe label precautions.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

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

Keep away from heat and sources of ignition. Keep container tightly closed in a dry and wellventilated place.

Recommended storage temperature see product label.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Engineering measures

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

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:	polychloroprene
Glove thickness:	0.65 mm
Break through time:	> 120 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 720 Camapren® (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

Flame retardant antistatic protective clothing

Respiratory protection required when vapours/aerosols are generated.

Recommended Filter type: filter ABEK

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.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	aromatic
Odour Threshold	No information available.
pH	5 - 7 at 10 g/l 20 °C
Melting point	No information available.
Boiling point	No information available.
Flash point	15 °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	0.89 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	at 20 °C soluble
Partition coefficient: noctanol/water	No information available.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

Vapours may form explosive mixture with air.

10.2 Chemical stability

heat-sensitive
sensitive to frost

10.3 Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapours with:

Alkali metals, Alkaline earth metals,
Aluminium

Exothermic reaction

with:

Oxidizing agents, Aldehydes, Amines, fuming sulfuric acid,
Iron

Risk of explosion

with:

chlorates, Phosgene, organic nitro compounds, hydrogen peroxide, nitrogen oxides

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Mixture

Acute oral toxicity

LD50 rat: 500 - 2,000 mg/kg (External MSDS)

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

Acute inhalation toxicity

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

Acute dermal toxicity

This information is not available.

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
Target Organs: Central nervous system
Mixture may cause drowsiness or dizziness.

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

Hexadecyltrimethylammonium chloride

Acute oral toxicity

Acute toxicity estimate: 500.1 mg/kg

Expert judgement

2-Propanol

Acute oral toxicity

LDLO human: 3,570 mg/kg (RTECS)

LD50 rat: 5,045 mg/kg (RTECS)

Acute inhalation toxicity

LC50 rat: 46.5 mg/l; 4 h (External MSDS)

Acute dermal toxicity

LD50 rabbit: 12,800 mg/kg (RTECS)

Eye irritation

rabbit

Result: Eye irritation

(RTECS)

Sensitisation

Sensitisation test: guinea pig

Result: negative

(IUCLID)

Germ cell mutagenicity

Genotoxicity in vivo

Mutagenicity (mammal cell test): micronucleus.

Result: negative

(IUCLID)

Genotoxicity in vitro

Ames test

Result: negative

(IUCLID)

Carcinogenicity

Did not show carcinogenic effects in animal experiments. (IUCLID)

Reproductive toxicity

No impairment of reproductive performance in animal experiments. (IUCLID)

Teratogenicity

Did not show teratogenic effects in animal experiments. (IUCLID)

SECTION 12. Ecological information

Mixture

12.1 Toxicity

Toxicity to fish

LC50 Danio rerio (zebra fish): 0.6 mg/l; 96 h (External MSDS)

Toxicity to bacteria

EC50 Pseudomonas putida: 3 mg/l DIN
38412 (External MSDS)

12.2 Persistence and degradability

Biodegradability

> 80 %

OECD Test Guideline 302B

(External MSDS)

Readily eliminated from water

Chemical Oxygen Demand (COD)

1.566 mg/g

(External MSDS)

12.3 Bioaccumulative potential

No information available.

12.4 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.

12.5 Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

Components

Hexadecyltrimethylammonium chloride

No information available.

2-Propanol

Toxicity to fish

LC50 *Lepomis macrochirus* (Bluegill sunfish): 1,400 mg/l; 96 h (ECOTOX Database)

Toxicity to daphnia and other aquatic invertebrates

EC50 *E.sulcatum*: 4,930 mg/l; 72 h (maximum permissible toxic concentration) (Lit.)

EC50 *Daphnia magna* (Water flea): 13,299 mg/l; 48 h (IUCLID)

Toxicity to algae

IC50 *Desmodesmus subspicatus* (green algae): > 1,000 mg/l; 72 h (IUCLID)

Toxicity to bacteria

EC50 *Pseudomonas putida*: 1,050 mg/l; 16 h (Lit.)

Biodegradability

95%; 21 d

OECD Test Guideline 301E

Readily biodegradable.

Theoretical oxygen demand (ThOD)

2,400 mg/g

(Lit.)

Ratio BOD/ThBOD

BOD5 49 %

(IUCLID)

Ratio COD/ThBOD

95 %

(Lit.)

SECTION 13. Disposal considerations

Waste treatment methods

Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.