

Chemical Safety Data Sheet MSDS / SDS

Benzyltrimethylammonium chloride SDS

Revision Date:2024-04-25 Revision Number:1

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SECTION 1: Identification of the substance/mixture and of the company/undertaking**Product identifier**

Product name: Benzyltrimethylammonium chloride

CAS: 56-93-9

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

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

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SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 3, Oral

Acute toxicity - Category 3, Dermal

Acute toxicity - Category 4, Inhalation
Germ cell mutagenicity, Category 2
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H301 Toxic if swallowed
H311 Toxic in contact with skin
H332 Harmful if inhaled
H341 Suspected of causing genetic defects
H412 Harmful to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P203 Obtain, read and follow all safety instructions before use.
P273 Avoid release to the environment.

Response

P301+P316 IF SWALLOWED: Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P316 Get emergency medical help immediately.
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P317 Get medical help.
P318 IF exposed or concerned, get medical advice.

Storage

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients**Substance**

Chemical name: Benzyltrimethylammonium chloride

Common names and synonyms: Benzyltrimethylammonium chloride

CAS number: 56-93-9

EC number: 200-300-3

Concentration: 100%

SECTION 4: First aid measures**Description of necessary first-aid measures****If inhaled**

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms/effects, acute and delayed

Ingestion causes gastrointestinal disturbances. Contact with liquid irritates eyes and may irritate skin. (USCG, 1999)

Indication of immediate medical attention and special treatment needed, if necessary

no data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Wear goggles and self-contained breathing apparatus. Extinguish with dry chemical, foam or carbon dioxide. Water may be ineffective on fire.

Specific hazards arising from the chemical

Special Hazards of Combustion Products: Toxic oxides of nitrogen and hydrochloric acid fumes may form in fire. (USCG, 1999)

Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must

be avoided.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Solid. Crystalline.
Colour:	Colorless.
Odour:	Mild almond odor
Melting point/freezing point:	< -50 °C. Remarks:Sax, but not Lewis, mentions that this is for a 61% solution in water.
Boiling point or initial boiling point and boiling range:	> 135 °C. Remarks:Stable up to 135 C, above which benzyl chloride and trimethylamine are formed.
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	24°C(lit.)
Auto-ignition temperature:	> 400 °C. Remarks:No endothermic or exothermic reaction between 23°C and 401°C.

Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 10.2. Temperature:20°C. Remarks:Std dev. of 5 measurements: 5.48 E-02 mPas.
Solubility:	>27.9 [ug/mL]
Partition coefficient n-octanol/water:	log Pow = -2.17. Temperature:25 °C. Remarks:Determined from a 60 wt% aqueous solution, pH not reported.
Vapour pressure:	0 hPa. Temperature:25 °C. Remarks:Estimated value from MPBPWin v1.41 program.
Density and/or relative density:	1.133 g/cm ³ . Temperature:23 °C.;1.133. Temperature:23 °C.;Ca. 500 kg/m ³ .
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

Stable up to 135 deg c, above which benzyl chloride & trimethylamine are formed

Possibility of hazardous reactions

BENZYLTRIMETHYLAMMONIUM CHLORIDE can react with oxidizing materials (NTP, 1992). Toxic oxides of nitrogen and hydrochloric acid fumes may form in fire (USCG, 1999). Quaternary ammonium salts often serve as catalysts in reactions. They are incompatible with many strong oxidizers and reducing agents, such as metal hydrides, alkali/active metals, and organometallics. Unlike the ammonium ion, [NH₄]⁺, and the primary, secondary, or tertiary ammonium cations, the quaternary ammonium cations are permanently charged, independent of the pH of their solution.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits very toxic fumes of /hydrogen chloride and nitrogen oxides/.

SECTION 11: Toxicological information**Acute toxicity**

Oral: no data available

Inhalation: LC50 - rat (male/female) - ca. 1.14 mg/L air.

Dermal: LD50 - rabbit (male/female) - 510 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information**Toxicity**

Toxicity to fish: LC50 - *Oryzias latipes* - > 1 000 mg/L - 48 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia pulex* - 11.94 mg/L - 48 h.

Toxicity to algae: NOEC - *Oscillatoria* sp. - > 0.001 mol/L - 14 d.

Toxicity to microorganisms: EC50 - activated sludge of a predominantly domestic sewage - > 1 000 mg/L - 3 h. Remarks:Respiration rate.

Persistence and degradability

At an initial concentration of 100 mg/L, trimethylbenzylammonium chloride did not biodegrade when incubated with activated sludge for ten days(1), although at high concentrations it may be toxic to the microbial population(2). Studies on the influence of chemical structure on quaternary ammonium compound (QACs) biodegradability suggest that alkyltrimethylammonium QACs will be most rapidly degraded followed by alkyldimethylbenzylammonium and alkyipyridinium QACs; few, if any, of the QACs should be regarded as persistent(2). The acclimation of the microbial community may profoundly influence the biodegradability of alkyldimethylbenzylammonium QACs(2).

Bioaccumulative potential

A BCF of <0.2 was measured for trimethylbenzylammonium(1). According to a classification scheme(2), this BCF suggests the

potential for bioconcentration in aquatic organisms is low.

Mobility in soil

The Koc of trimethylbenzylammonium chloride is estimated as 900(SRC), using a log Kow of -2.17(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that trimethylbenzylammonium chloride is expected to have low mobility in soil. Quaternary ammonium compounds (QACs) are strongly adsorbed by a wide variety of materials, and alkyl dimethylbenzylammonium QACs are known to adsorb strongly to sewage sludge(4).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: no data available

IMDG: no data available

IATA: no data available

UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: III (For reference only, please check.)

IMDG: III (For reference only, please check.)

IATA: III (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any