Benzyltrimethylammonium chloride



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

1.1. Product identifier

Trade name

Benzyltrimethylammonium chloride

CAS number

56-93-9

EC number

200-300-3

Synonyms

N,N,N-trimethyl(phenyl)methanaminium chloride

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

Research and development.

Not suitable for use in

Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier

Molekula Group

Street address

Molekula Ltd, Lingfield Way, Darlington,

DL1 4XX Darlington

United Kingdom

Telephone

+44 (0) 3302 000 333

Email

info@molekula.com

Web site

www.molekula.com

Contact person

Kevin Banks

Email address

+44 (0) 7769276927

1.4. Emergency telephone number

Poison center/Additional emergency number

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

Benzyltrimethylammonium chloride



SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Classification

Acute toxicity, oral, hazard category 3
Acute toxicity, dermal, hazard category 3
Acute toxicity, inhalation, hazard category 4
Germ cell mutagenicity, hazard category 2
Hazardous to the aquatic environment — Chronic hazard category 3

Hazard statements

H301 + H311, H332, H341, H412

Supplemental hazard statements

EUH070

2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms





Signal word

Danger

Hazard statements

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

Supplemental hazard statements

EUH070 Toxic by eye contact.

Benzyltrimethylammonium chloride



Precautionary statements

P201 Obtain special instructions before use.

P202 Do not handle until all safety precautions have been read and understood.

P260 Do not breathe dust/fumes/gas/mist/vapours/spray.

P264 Wash skin thoroughly after handling.

P271 Use only outdoors or in a well-ventilated area.

P273 Avoid release to the environment.

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

P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.

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

P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P308 + P313 IF exposed or concerned: Get medical advice/attention.

P312 Call a POISON CENTER/doctor if you feel unwell.

P330 Rinse mouth.

P361 + P364 Take off immediately all contaminated clothing and wash it before reuse.

P405 Store locked up.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.2. Mixtures

Chemical name	CAS No. EC No. REACH No. Index No.	Concentration	Classification	H-phrase M factor acute M factor chronic	Note
Benzyltrimethylammonium chloride	56-93-9 200-300-3 - -	100%	Acute Tox. 3 - oral, Acute Tox. 3 - dermal, Acute Tox. 4 - inhalation, Muta. 2, Aquatic Chronic 3	H301 + H311, H332, H341, H412 -	-

Molecular weight

185.69

Substance additional information

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

IF exposed or concerned: Get medical advice/attention. First aiders/ medical personnel need to protect themselves. Show this Safety Data Sheet (SDS) to medical personnel.

Benzyltrimethylammonium chloride



Inhalation

Toxic if inhaled. IF INHALED: Remove person to fresh air and keep comfortable for breathing. Maintain an open airway. Loosen any tight clothing, such as a collar, tie or belt. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. If breathing stops, provide artificial respiration. Place unconscious person on the side in the recovery position and ensure breathing can take place. Get medical attention. Immediately call a POISON CENTER/doctor.

Skin contact

In case of skin contact: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower]. Immediately call a POISON CENTER/doctor.

Eye contact

Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

Ingestion

IF SWALLOWED: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only if the persons are fully conscious and awake). NEVER MAKE AN UNCONSCIOUS PERSON VOMIT OR DRINK FLUIDS! Place unconscious person on the side in the recovery position and ensure breathing can take place. NOTE! Effects may be delayed. Keep affected person under observation.

Information for doctors

It may be dangerous for first aid personnel to carry out mouth-to-mouth resuscitation.

4.2. Most important symptoms and effects, both acute and delayed

The severity of the symptoms described will vary dependant of the concentration and the length of exposure. See section 11 for more detailed information on health effects and symptoms.

<u>Inhalation</u>

Single exposure may cause the following adverse effects: Difficulty in breathing. Headache. Exhaustion and weakness.

Skin contact

Single exposure may cause the following adverse effects: Pain.

Eye contact

Single exposure may cause the following adverse effects: Severe irritation. Unconsciousness, possibly death.

Ingestion

Single exposure may cause the following adverse effects: Severe abdominal pain. May cause severe internal injury.

4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically. No special treatment requirement.

Benzyltrimethylammonium chloride



SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish. Use fire-extinguishing media appropriate for surrounding materials.

Unsuitable extinguishing media

Do not use water jet as an extinguisher, as this will spread the fire.

5.2. Special hazards arising from the substance or mixture

Specific hazards:

This product is toxic.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon monoxide (CO). Carbon dioxide (CO2).

Nitrous gases (NOx).

Hydrogen chloride (HCI).

5.3. Advice for firefighters

Special protective equipment for fire-fighters

Avoid breathing gas, fume, vapours or spray. Evacuate area. Cool containers exposed to heat with water spray and remove container, if no risk is involved. Avoid discharge to the aquatic environment. Keep run-off water out of sewers and water sources. Dike for water control. If risk of water pollution occurs, notify appropriate authorities.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For personal protection, see section 8. DO NOT touch spilled material. Avoid inhalation of dust and contact with skin and eyes. Provide adequate ventilation.

6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground.

6.3. Methods and material for containment and cleaning up

Provide adequate ventilation. Wear protective clothing, gloves, eye and face protection. Collect spillage with shovel, broom or the like and reuse, if possible. Dispose of large amounts of spillage/waste according to agreement with local authorities. Wash thoroughly after dealing with a spillage.

6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Preventive handling precautions

For precautions see section 2.2.

Benzyltrimethylammonium chloride



General hygiene

Wash skin thoroughly after handling.

7.2. Conditions for safe storage, including any incompatibilities

Store at room temperature. Store in a dry place. Store in a closed container.

Air sensitive. Store contents under inert gas.

Storage class Toxic storage.

7.3. Specific end use(s)

No specific usage precautions noted.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Exposure limits

TWA

STEL

8.2. Exposure controls

Eye / face protection

Wear eye protection.

Hand protection

Wear protective gloves. Recommended gloves: Nitrile.

Glove Thickness: 0.11mm Breakthrough time: 8 hours

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals. Wash contaminated skin thoroughly after handling.

Other skin protection

Wash skin thoroughly after handling.

Respiratory protection

Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

Environmental exposure controls

Avoid discharge into drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state

Solid

Benzyltrimethylammonium chloride



Colour

White / off-white.

<u>Odour</u>

Characteristic.

Melting point / freezing point

239

Boiling point or initial boiling point and boiling range

No data available

Flammability

No data available

Lower and upper explosion limit

No data available

Flash point

No data available

Auto-ignition temperature

No data available

Decomposition temperature

No data available

<u>рН</u>

6-8

Kinematic viscosity

No data available

Solubility

No data available

Water solubility

800 g/l water @ 20°C

Partition coefficient n-octanol/water

log Pow: -2.17 - Bioaccumulation is not expected., (Lit.)

Vapour pressure

<0.0001 hPa

Density and/or relative density

No data available

Relative density

1.133

Benzyltrimethylammonium chloride



Relative vapour density

No data available

Particle characteristics

No data available

9.2. Other information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

No data available

10.2. Chemical stability

Stable under normal temperature conditions. Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Violent reactions possible with:

Alkalis

oxidising agents

10.4. Conditions to avoid

Keep at temperature not exceeding 135 □

10.5. Incompatible materials

Strong alkalis. Strong oxidising agents.

10.6. Hazardous decomposition products

See section 5.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008 <u>Acute toxicity</u>

Product / Sub- stance name CAS / EC no.	Dose descriptor	Value / Dose	Exposure route	Duration of expos- ure	Test animals
Benzyltrimethylam- monium chloride 56-93-9 / 200-300-3	LD50	125-250mg/kg	-	-	Rat
Benzyltrimethylam- monium chloride 56-93-9 / 200-300-3	LC50	1.14mg/l	dust	4 hours	Rat
Benzyltrimethylam- monium chloride	Acute Toxicity (Dermal LD50):	510mg/kg	-	-	Rabbit

Benzyltrimethylammonium chloride



Product / Sub- stance name CAS / EC no.	Dose descriptor	Value / Dose	Exposure route	Duration of expos- ure	Test animals
56-93-9 / 200-300-3					

Skin corrosion/irritation

Product / Substance name CAS / EC no.	Result	Duration of exposure	Species
Benzyltrimethylammonium chloride 56-93-9 / 200-300-3	slight irritation	24 hours	Rabbit

Serious eye damage/irritation

Product / Substance name CAS / EC no.	Result	Species
Benzyltrimethylammonium chloride 56-93-9 / 200-300-3	No eye irritation.	Rabbit

Respiratory or skin sensitisation

Product / Substance name CAS / EC no.	Result	Species	Method / Guideline
Benzyltrimethylammonium chloride 56-93-9 / 200-300-3	Negative.	Mouse	Local Lymph Node Assay

Germ cell mutagenicity

Product / Sub- stance name CAS / EC no.	Result	Exposure route	Metabolic activa- tion / Exposure	Species	Method / Guideline
Benzyltrimethylam- monium chloride 56-93-9 / 200-300-3	Negative.	-	with and without metabolic activation	Salmonella typh- imurium	Ames test
Benzyltrimethylam- monium chloride 56-93-9 / 200-300-3	Positive results were obtained in some in vitro tests.	-	with and without metabolic activation	Chinese hamster lung cells	Chromosome aberration:
Benzyltrimethylam- monium chloride 56-93-9 / 200-300-3	Negative.	-	with and without metabolic activation	Chinese Hamster cells: Ovary	In vitro mammalian cell gene mutation test.

Benzyltrimethylammonium chloride



Product / Sub- stance name CAS / EC no.	Result	Exposure route	Metabolic activa- tion / Exposure	Species	Method / Guideline
Benzyltrimethylam- monium chloride 56-93-9 / 200-300-3	Positive.	Oral	-	Mouse Red blood cells (erythrocytes)	Mutagenicity (mammal cell test): Micronucleus test

Aspiration hazard

Based on available data, the classification criteria are not met.

11.2. Information on other hazards

No data available

SECTION 12: Ecological information

12.1. Toxicity <u>Acute fish toxicity</u>

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
Benzyltrimethylam- monium chloride 56-93-9 / 200-300-3	LC50	1000mg/l	48 hours	Oryzias latipes (Red killifish)
Benzyltrimethylam- monium chloride 56-93-9 / 200-300-3	LC50	1000mg/l	48 hours	Oryzias latipes (Red killifish)

Acute crustacean toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
Benzyltrimethylam- monium chloride 56-93-9 / 200-300-3	EC50	11.94 mg/l	48 hours	water flea
Benzyltrimethylam- monium chloride 56-93-9 / 200-300-3	EC50	11.94 mg/l	48 hours	water flea

Micro-/macro organism toxicity

Benzyltrimethylammonium chloride



Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure
Benzyltrimethylammonium chloride 56-93-9 / 200-300-3	aerobic	1% Not readily biodegradable	28 days
Benzyltrimethylammonium chloride 56-93-9 / 200-300-3	aerobic	1% Not readily biodegradable	28 days

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

No data available

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

No data available

12.6. Endocrine disrupting properties

No data available

12.7. Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal considerations

Dispose of contents/container in accordance with local regulations.

SECTION 14: Transport information

14.1. UN number

2811

14.2. UN proper shipping name

ADR / RID / ADN proper shipping name

TOXIC SOLID, ORGANIC, N.O.S. (Benzyltrimethylammonium chloride)

IMDG proper shipping name

TOXIC SOLID, ORGANIC, N.O.S. (Benzyltrimethylammonium chloride)

IATA proper shipping name

Toxic solid, organic, n.o.s. (Benzyltrimethylammonium chloride)

Benzyltrimethylammonium chloride



14.3. Transport hazard class(es)

<u>Label</u>

ADR/RID/ADN



6.1

IMDG



6.1

IATA



6.1

ADR / RID Class

6.1

ADR / RID Classification code

T2

ADR / RID hazard identification number

60

IMDG Class

6 1

IATA Class

6.1

ADN Class

6.1

ADN Class Code

T2

14.4. Packing group

ADR / RID / ADN: III

IMDG: III IATA: III

Benzyltrimethylammonium chloride



14.5. Environmental hazards

IMDG EmS

F-A, S-A

14.6. Special precautions for user

Tunnel restriction code: E Transport category: 2

14.7. Maritime transport in bulk according to IMO instruments

IBC Instruction: IBC08

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture <u>EU regulations</u>

This material safety data sheet complies with the requirements of Regulation (EU) 2020/878.

National regulations

No data available

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

SECTION 16: Other information

Phrase meaning

Acute Tox. 3 - oral - Acute toxicity, oral, hazard category 3

Acute Tox. 3 - dermal - Acute toxicity, dermal, hazard category 3

Acute Tox. 4 - inhalation - Acute toxicity, inhalation, hazard category 4

Muta. 2 - Germ cell mutagenicity, hazard category 2

Aquatic Chronic 3 - Hazardous to the aquatic environment — Chronic hazard category 3

H301 + H311 Toxic if swallowed or in contact with skin

H332 Harmful if inhaled.

H341 Suspected of causing genetic defects.

H412 Harmful to aquatic life with long lasting effects.

EUH070 Toxic by eye contact.