

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

Benzyltrimethylhexadecylammonium chloride



Version number: 2

Issued: 2024-02-20

Replaces SDS: 2019-08-19

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

1.1. Product identifier

Trade name

Benzyltrimethylhexadecylammonium chloride

CAS number

122-18-9

EC number

204-526-3

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

Relevant identified uses

Research and development. Laboratory Chemicals. Manufacture of substances.

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

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

+44 (0) 7769276927

1.4. Emergency telephone number

Poison center/Additional emergency number

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

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SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Classification

Serious eye damage, hazard category 1

Hazardous to the aquatic environment — Acute hazard category 1

Hazardous to the aquatic environment — Chronic hazard category 1

Skin corrosion, hazard category 1B

Acute toxicity, oral, hazard category 4

Hazard statements

H302, H314, H318, H400, H410

2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms



Signal word

Danger

Hazard statements

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H410 Very toxic to aquatic life with long lasting effects.

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Precautionary statements

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

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P273 Avoid release to the environment.

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

P310 Immediately call a POISON CENTER/doctor.

P321 Specific treatment (see on this label).

P330 Rinse mouth.

P363 Wash contaminated clothing before reuse.

P391 Collect spillage.

P301 + P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.

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

P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

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

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

P405 Store locked up.

P501 Dispose of contents/container to local regulations.

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-phrases M factor acute M factor chronic	Note
Benzyltrimethylhexadecylamm onium chloride	122-18-9 204-526-3 - -	100%	Acute Tox. 4 - oral, Skin Corr. 1B, Eye Dam. 1, Aquatic Acute 1, Aquatic Chronic 1	H302, H314, H318, H400, H410 - -	-

Molecular weight

396.09

Substance additional information

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

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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.

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor. If breathing stops, provide artificial respiration. For breathing difficulties oxygen may be necessary.

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). Administer activated charcoal (20 - 40g in a 10% slurry) and consult a doctor as quickly as possible. Do not attempt to neutralise.

Information for doctors

No data available.

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. Causes burns by all exposure routes.

See section 11 for more detailed information on health effects and symptoms.

Inhalation

Single exposure may cause the following adverse effects: Causes severe burns. Difficulty in breathing. Unconsciousness, possibly death.

Skin contact

Single exposure may cause the following adverse effects: Causes severe burns. Blistering may occur. May be absorbed in the body and cause dizziness, nausea and vomiting. Unconsciousness, death.

Eye contact

Single exposure may cause the following adverse effects: Causes serious eye damage. Unconsciousness, possibly death.

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Ingestion

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

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

Treat symptomatically. Immediately call a POISON CENTER/doctor.

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.

Unsuitable extinguishing media

No specific fire fighting procedure given.

5.2. Special hazards arising from the substance or mixture

Specific hazards: Corrosive.

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

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

Nitrous gases (NO_x).

Hydrogen Chloride gas

Combustible.

Vapours are heavier than air and may spread near ground to sources of ignition.

Forms explosive mixtures with air on intense heating.

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

5.3. Advice for firefighters

Special protective equipment for fire-fighters

Evacuate area. Avoid breathing gas, fume, vapours or spray. Prevent skin contact by maintaining a safe distance and by wearing suitable protective equipment/ clothing. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Do not breathe vapour/spray. Avoid contact with skin and eyes. For personal protection, see section 8.

In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.

6.2. Environmental precautions

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

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6.3. Methods and material for containment and cleaning up

Collect with absorbent, non-combustible material into suitable containers.

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. Work under hood. Take action to prevent static discharges. Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Avoid ingestion and inhalation.

General hygiene

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Wash contaminated skin thoroughly after handling. Do not eat, drink or smoke when using this product. Remove contaminated clothing and launder thoroughly before re-use.

7.2. Conditions for safe storage, including any incompatibilities

Store in a dry place. Store in a closed container.

Store at ambient temperature.

Protect from moisture. Store contents under inert gas.

7.3. Specific end use(s)

No specific usage precautions noted.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No data available

8.2. Exposure controls

Personal Protective Equipment Symbols



Eye / face protection

Wear eye protection.

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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

Colour

White.

Odour

Aromatic.

Melting point / freezing point

54 - 65 °C

Boiling point or initial boiling point and boiling range

163 °C

Flammability

No data available

Lower and upper explosion limit

No data available

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Flash point

62 °C

Auto-ignition temperature

No data available

Decomposition temperature

No data available

pH

5.55

Kinematic viscosity

No data available

Solubility

5 - 8.5 g/l

Partition coefficient n-octanol/water

log Pow: 3.02 at 25 °C - Bioaccumulation is not expected.

Vapour pressure

No data available

Density and/or relative density

0.4826 - 0.5064 g/cm³

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

Forms explosive mixtures with air on intense heating.

15 (approx) Kelvin below the flash point is to be rated as critical.

The following applies in general to flammable organic substances and mixtures: when finely distributed, the risk of a dust explosion may be assumed.

10.2. Chemical stability

Stable under the prescribed storage conditions. Hygroscopic.

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10.3. Possibility of hazardous reactions

No data available

10.4. Conditions to avoid

strong heating Moisture.

10.5. Incompatible materials

Strong oxidising agents.
finely Powdered metal.
Acids.
Bases.

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

Acute toxicity

Product / Substance name CAS / EC no.	Dose descriptor	Value / Dose	Exposure route	Test animals
Benzyltrimethylhexa- decylammonium chlor- ide 122-18-9 / 204-526-3	LD50	1250 mg/kg	Oral	Rat

Skin corrosion/irritation

Product / Substance name CAS / EC no.	Result	Species
Benzyltrimethylhexadecylammonium chloride 122-18-9 / 204-526-3	CAUSES BURNS.	Mouse

Serious eye damage/irritation

Product / Substance name CAS / EC no.	Result
Benzyltrimethylhexadecylammonium chloride	Causes serious eye damage.

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Product / Substance name CAS / EC no.	Result
122-18-9 / 204-526-3	

Germ cell mutagenicity

Product / Substance name CAS / EC no.	Result	Metabolic activation / Exposure	Species	Method / Guideline
Benzyltrimethylhexa- decylammonium chlor- ide 122-18-9 / 204-526-3	Negative.	with and without meta- bolic activation	S. typhimurium	Ames 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

Acute fish toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
Benzyltrimethylhexa- decylammonium chlor- ide 122-18-9 / 204-526-3	EC50	0.02 mg/l	48 hours	Daphnia magna

Micro-/macro organism toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
Benzyltrimethylhexa- decylammonium chlor-	EC50	0.22 mg/l	30 minutes	Photobacterium phos- phoreum

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Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
ide 122-18-9 / 204-526-3				

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

This product does not contain any known or suspected endocrine disruptors.

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/regional/national/international regulations.

SECTION 14: Transport information

14.1. UN number

3261

14.2. UN proper shipping name

ADR / RID / ADN proper shipping name

CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (Benzyltrimethylhexadecylammonium chloride)

IMDG proper shipping name

CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (Benzyltrimethylhexadecylammonium chloride)

IATA proper shipping name

Corrosive solid, acidic, organic, n.o.s. (Benzyltrimethylhexadecylammonium chloride)

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14.3. Transport hazard class(es)

Label

ADR/RID/ADN



8

Environmental hazard



IMDG



8

Environmental hazard



IATA



8

Environmental hazard



ADR / RID Class

8

ADR / RID Classification code

C4

ADR / RID hazard identification number

80

IMDG Class

8

IATA Class

8

ADN Class

8

ADN Class Code

C4

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14.4. Packing group

ADR / RID / ADN: III
 IMDG: III
 IATA: III

14.5. Environmental hazards

Not applicable

14.6. Special precautions for user

Special precautions for user

Tunnel restriction code: E
 Transport category: 3

IMDG EmS

F-A, S-B

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

EU regulations

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.
 This material safety data sheet complies with the requirements of Regulation (EU) 2020/878.

National regulations

Directive: 2012/18/EU: ENVIRONMENTAL HAZARDS

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

SECTION 16: Other information

Phrase meaning

Eye Dam. 1 - Serious eye damage, hazard category 1
 Aquatic Acute 1 - Hazardous to the aquatic environment — Acute hazard category 1
 Aquatic Chronic 1 - Hazardous to the aquatic environment — Chronic hazard category 1
 Skin Corr. 1B - Skin corrosion, hazard category 1B
 Acute Tox. 4 - oral - Acute toxicity, oral, hazard category 4
 H302 Harmful if swallowed.
 H314 Causes severe skin burns and eye damage.
 H318 Causes serious eye damage.
 H400 Very toxic to aquatic life.
 H410 Very toxic to aquatic life with long lasting effects.