

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

Hexadecyltrimethylammonium bromide



Version number: 2

Issued: 2024-04-18

Replaces SDS: 2022-02-08

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

1.1. Product identifier

Trade name

Hexadecyltrimethylammonium bromide

CAS number

57-09-0

EC number

200-311-3

Synonyms

Cetyltrimethylammonium bromide

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

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www.molekula.com

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1.4. Emergency telephone number

Poison center/Additional emergency number

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

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 irritation, hazard category 2
 Specific Target Organ Toxicity — Repeated exposure, hazard category 2
 Acute toxicity, oral, hazard category 4
 Specific Target Organ Toxicity — Single exposure, hazard category 3

Hazard statements

H302, H315, H318, H335, H373, 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.
 H315 Causes skin irritation.
 H318 Causes serious eye damage.
 H335 May cause respiratory irritation.
 H373 May cause damage to organs through prolonged or repeated exposure.
 H410 Very toxic to aquatic life with long lasting effects.

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Precautionary statements

P202 Do not handle until all safety precautions have been read and understood.
P261 Avoid breathing dust/fumes/gas/mist/vapours/spray.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P272 Contaminated work clothing should not be allowed out of the workplace.
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.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P312 Call a POISON CENTER/doctor if you feel unwell.
P314 Get medical advice/attention if you feel unwell.
P330 Rinse mouth.
P332 + P313 If skin irritation occurs: Get medical advice/attention.
P337 + P313 If eye irritation persists: Get medical advice/attention.
P362 + P364 Take off contaminated clothing and wash it before reuse.
P391 Collect spillage.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
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
Hexadecyltrimethylammonium bromide	57-09-0 200-311-3 - -	100%	Acute Tox. 4 - oral, Skin Irrit. 2, Eye Dam. 1, STOT RE 2, Aquatic Acute 1, Aquatic Chronic 1, STOT SE 3	H302, H315, H318, H335, H373, H400, H410 - -	-

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Molecular weight

364.45

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.

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.

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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.

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. Combustible.

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 bromide gas

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.

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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.

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.

Moisture Sensitive. Store 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

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8.2. Exposure controls

Personal Protective Equipment Symbols



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

Colour

White.

Odour

Slight odour.

Melting point / freezing point

237 - 251 °C

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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

244 °C

Auto-ignition temperature

210 °C

Decomposition temperature

No data available

pH

5 - 7

Kinematic viscosity

No data available

Solubility

No data available

Water solubility

36.4 g/l

Partition coefficient n-octanol/water

log Pow: 2.26 - (Lit.), Bioaccumulation is not expected.

Vapour pressure

No data available

Density and/or relative density

2.3 g/cm³

Relative vapour density

No data available

Explosive properties

Not classified as explosive.

Particle characteristics

No data available

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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.

10.2. Chemical stability

Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidising agents.

Caution! In contact with nitrites, nitrates, nitrous acid possible liberation of nitrosamines!

10.4. Conditions to avoid

strong heating

10.5. Incompatible materials

Strong oxidising agents. Strong bases Strong acids.

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
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	LD50	1550 mg/kg	Oral	Rat
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	LD50	2150 mg/kg	Dermal	Rabbit

Skin corrosion/irritation

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Product / Substance name CAS / EC no.	Result	Duration of exposure	Species
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	Irritating to skin	24 hours	Rabbit

Serious eye damage/irritation

Product / Substance name CAS / EC no.	Result	Species
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	Causes serious eye damage.	Rabbit

Respiratory or skin sensitisation

Product / Substance name CAS / EC no.	Result	Species	Method / Guideline
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	Negative.	Guinea Pig	Maximization Test

STOT-single exposure

Product / Substance name CAS / EC no.	Exposure route	Result
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	Inhalation.	May cause respiratory irritation.

STOT-repeated exposure

Product / Substance name CAS / EC no.	Exposure route	Result
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	Oral	May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard

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

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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
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	LC50	0.2 mg/l	96 hours	Brachydanio rerio (Zebra Fish)

Acute algae toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	NOEC	0.001 mg/l	72 hours	Desmodesmus subspicatus (green algae)
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	ErC50	0.00411 mg/l	72 hours	Pseudokirchneriella subcapitata

Acute crustacean toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	EC50	0.037 mg/l	48 hours	Daphnia magna

Micro-/macro organism toxicity

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Product / Substance name CAS / EC no.	Measurement type	Value / Result	Species
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	EC50	19 mg/l	Activated sludge.

Chronical toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	NOEC	0.023 mg/l	21 days	Daphnia magna

12.2. Persistence and degradability

Persistence and degradability

Product / Substance name CAS / EC no.	Type of test	Duration	Result	Degradation
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	aerobic	11 days	100%	The product is readily biodegradable.

12.3. Bioaccumulative potential

Bioaccumulative potential

Product / Substance name CAS / EC no.	Bioconcentration factor (BCF)	Duration	Result	Species
Hexadecyltrimethylammonium bromide 57-09-0 / 200-311-3	407 - 741	8 weeks	0.05 mg/l	Cyprinus carpio (Common carp)

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

No data available

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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

3077

14.2. UN proper shipping name

ADR / RID / ADN proper shipping name

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Hexadecyltrimethylammonium bromide)

IMDG proper shipping name

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Hexadecyltrimethylammonium bromide)

IATA proper shipping name

Environmentally hazardous substance, solid, n.o.s. (Hexadecyltrimethylammonium bromide)

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14.3. Transport hazard class(es)

Label

ADR/RID/ADN



9

Environmental hazard



IMDG



9

Environmental hazard



IATA



9

Environmental hazard



ADR / RID Class

9

ADR / RID Classification code

M7

ADR / RID hazard identification number

90

IMDG Class

9

IATA Class

9

ADN Class

9

ADN Class Code

M7

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14.4. Packing group

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

14.5. Environmental hazards

Environmental hazards

ADR/RID/ADN: Hazardous for the environment

14.6. Special precautions for user

Special precautions for user

Tunnel restriction code: -
 Transport category: 3

IMDG EmS

F-A, S-F

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: E1 ENVIRONMENTAL HAZARDS

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

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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 Irrit. 2 - Skin irritation, hazard category 2

STOT RE 2 - Specific Target Organ Toxicity — Repeated exposure, hazard category 2

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

STOT SE 3 - Specific Target Organ Toxicity — Single exposure, hazard category 3

H302 Harmful if swallowed.

H315 Causes skin irritation.

H318 Causes serious eye damage.

H335 May cause respiratory irritation.

H373 May cause damage to organs through prolonged or repeated exposure.

H400 Very toxic to aquatic life.

H410 Very toxic to aquatic life with long lasting effects.