

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.3 Revision Date 13.01.2021 Print Date 07.06.2022

GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

1.1 Product identifiers

Product name : Hexadecyltrimethylammonium bromide

Product Number : H5882 Brand : Sigma

REACH No. : 01-2119989160-35-XXXX

CAS-No. : 57-09-0

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

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Pte Ltd

(Co. Registration No. 199403788W)

2 Science Park Drive #05-01/12 Ascent Building

SINGAPORE 118222

SINGAPORE

Telephone : +65 6890 6633 Fax : +65 6890 6639

E-mail address : TechnicalService@merckgroup.com

1.4 Emergency telephone

Emergency Phone # : 1-800-262-8200

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Acute toxicity, Oral (Category 4), H302

Skin irritation (Category 2), H315

Serious eye damage (Category 1), H318

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335 Specific target organ toxicity - repeated exposure, Oral (Category 2), Gastrointestinal tract, H373

Short-term (acute) aquatic hazard (Category 1), H400 Long-term (chronic) aquatic hazard (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

A

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal word Danger

Hazard statement(s)

H302 Harmful if swallowed. H315 Causes skin irritation.

H318 Causes serious eye damage. H335 May cause respiratory irritation.

H373 May cause damage to organs (Gastrointestinal tract) through

prolonged or repeated exposure if swallowed.

H410 Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P273 Avoid release to the environment.

P280 Wear protective gloves/ eye protection/ face protection.
P301 + P312 Wear protective gloves/ eye protection/ face protection.
IF SWALLOWED: Call a POISON CENTER/ doctor if you feel

unwell.

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

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes.

Remove contact lenses, if present and easy to do. Continue

rinsing.

P314 Get medical advice/ attention if you feel unwell.

Supplemental Hazard

Statements

none

Reduced Labeling (<= 125 ml)

Pictogram

Signal word Danger

Hazard statement(s)

H318 Causes serious eye damage.

Precautionary statement(s)

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes.

Remove contact lenses, if present and easy to do. Continue

rinsing.

Supplemental Hazard

Statements

none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : Cetrimonium bromide

Palmityltrimethylammonium bromide

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CTAB

Cetyltrimethylammonium bromide

Formula : C19H42N.Br Molecular weight : 364,45 g/mol CAS-No. : 57-09-0 EC-No. : 200-311-3

Component		Classification	Concentration
N-Cetyl-N'N'N-trimethylammonium bromide			
CAS-No.	57-09-0	Acute Tox. 4; Skin Irrit. 2;	<= 100 %
EC-No.	200-311-3	Eye Dam. 1; STOT SE 3;	
		STOT RE 2; Aquatic Acute	
		1; Aquatic Chronic 1;	
		H302, H315, H318, H335,	
		H373, H400, H410	
		M-Factor - Aquatic Acute:	
		100 - Aquatic Chronic: 10	

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Water Foam Carbon dioxide (CO2) Dry powder

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Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NOx)

Hydrogen bromide gas

Combustible.

Vapors are heavier than air and may spread along floors.

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

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. 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: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated



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SECTION 8: Exposure controls/personal protection

8.1 **Control parameters**

Ingredients with workplace control parameters

8.2 Exposure controls

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

Skin protection

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).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: KCL 741 Dermatril® L

Body Protection

protective clothing

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a fullface particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type P2

The entrepeneur 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.

Control of environmental exposure

Do not let product enter drains.

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the US and Canada



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The life science business of Merck operates as MilliporeSigma in

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance Form: solid

Color: white

b) Odor weak

c) Odor Threshold No data available

d) pH 5,0 - 7 at 36,4 g/l at 25 °C

e) Melting point/range: 248 - 251 °C

point/freezing point

f) Initial boiling point No data available and boiling range

g) Flash point 244 °C - closed cup h) Evaporation rate No data available

i) Flammability (solid, No data available

gas)

j) Upper/lower No data available

flammability or explosive limits

k) Vapor pressure No data availablel) Vapor density No data available

m) Relative density 2,30 g/cm³

n) Water solubility 36,4 g/l at 20 °C - completely soluble

o) Partition coefficient: log Pow: 2,26 - (Lit.), Bioaccumulation is not expected.

n-octanol/water

p) Autoignition 210 °C temperature at 0,3 hPa

q) Decomposition No data available

temperature

r) Viscosity Viscosity, kinematic: No data available

Viscosity, dynamic: No data available

s) Explosive properties No data availablet) Oxidizing properties No data available

9.2 Other safety information

Surface tension 39 mN/m at 25 °C

SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating. A range from approx. 15 Kelvin below the flash point is to be rated as critical.

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The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

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

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - 1.550 mg/kg

(OECD Test Guideline 401)

Remarks:

(in analogy to similar products)

The value is given in analogy to the following substances: Hexadecyltrimethylammonium chloride

LD50 Dermal - Rabbit - male and female - 2.150 mg/kg

Remarks:

(in analogy to similar products)

(ECHA)

The value is given in analogy to the following substances: Hexadecyltrimethylammonium chloride

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h

Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage.

(OECD Test Guideline 405)

Remarks:

(in analogy to similar products)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Remarks:

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Aqueous solution

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is

identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Respiratory system

Specific target organ toxicity - repeated exposure

Oral - May cause damage to organs through prolonged or repeated exposure. -Gastrointestinal tract

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rabbit - male and female - Dermal - 28 d - LOAEL (Lowest observed adverse effect level) - 10 mg/kgRemarks: (in analogy to similar products)

Repeated dose toxicity - Rat - male and female - Oral - 28 d - NOAEL (No observed adverse effect level) - 100 mg/kgRemarks: (as aqueous solution)

(ECHA)

RTECS: BQ7875000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish semi-static test LC50 - Danio rerio (zebra fish) - 0,2 mg/l - 96 h

(OECD Test Guideline 203)

Toxicity to daphnia and other aquatic

semi-static test EC50 - Daphnia magna (Water flea) - 0,037 mg/l -

48 h

invertebrates (OECD Test Guideline 202)

Toxicity to algae static test ErC50 - Pseudokirchneriella subcapitata (green algae) -

> 0,00411 mg/l - 72 h (OECD Test Guideline 201)

static test NOEC - Desmodesmus subspicatus (green algae) - 0,001

mg/l - 72 h

(OECD Test Guideline 201)

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Toxicity to bacteria EC50 - activated sludge - 19 mg/l

Remarks: (ECHA)

12.2 Persistence and degradability

Biodegradability aerobic Chemical oxygen demand - Exposure time 11 d

Result: 100 % - Readily biodegradable.

(OECD Test Guideline 301E)

12.3 Bioaccumulative potential

Bioaccumulation Cyprinus carpio (Carp) - 8 Weeks

- 0,05 mg/l(N-Cetyl-N'N'N-trimethylammonium bromide)

Bioconcentration factor (BCF): 407 - 741

Due to the distribution coefficient n-octanol/water, accumulation in organisms is not expected.

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Other adverse effects

Very toxic to aquatic life.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 3077 IMDG: 3077 IATA: 3077

14.2 UN proper shipping name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (N-Cetyl-N'N'N-

trimethylammonium bromide)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (N-Cetyl-N'N'N-

trimethylammonium bromide)

IATA: Environmentally hazardous substance, solid, n.o.s. (N-Cetyl-N'N'N-

trimethylammonium bromide)

14.3 Transport hazard class(es)

ADR/RID: 9 IMDG: 9 IATA: 9

14.4 Packaging group

ADR/RID: III IMDG: III IATA: III

14.5 Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: yes

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14.6 Special precautions for user

Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

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

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

E1 ENVIRONMENTAL

HAZARDS

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 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 if swallowed.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

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Further information

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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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