

**SAFETY DATA SHEET**

according to Regulation (EC) No. 1907/2006

Version 6.8

Revision Date 24.02.2023

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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 for synthesis

Product Number : 8.14119  
Catalogue No. : 814119  
Brand : Millipore  
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 : Chemical for synthesis

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Chemie GmbH  
Eschenstrasse 5  
D-82024 TAUFKIRCHEN

Telephone : +49 (0)89 6513-1130  
Fax : +49 (0)89 6513-1161  
E-mail address : technischerservice@merckgroup.com

**1.4 Emergency telephone**

Emergency Phone # : 0800 181 7059 (CHEMTREC Deutschland)  
+49 (0)696 43508409 (CHEMTREC weltweit)

**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.



## 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	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.

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula : C<sub>19</sub>H<sub>42</sub>N.Br



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

Component	Classification	Concentration
<b>N-Cetyl-N'N'N-trimethylammonium bromide</b>		
CAS-No. 57-09-0 EC-No. 200-311-3	Acute Tox. 4; Skin Irrit. 2; 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	<= 100 %

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.



## 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Hydrogen bromide gas

Combustible.

Fire may cause evolution of:

hydrogen bromide, nitrogen oxides

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.

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## 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.

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## 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.

Recommended storage temperature see product label.

#### Storage class

Storage class (TRGS 510): 11: Combustible Solids

### 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](http://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

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](http://www.kcl.de)).

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 full-face 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).

##### **Control of environmental exposure**

Do not let product enter drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

- a) Physical state                      solid

Millipore- 8.14119

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The life science business of Merck operates as MilliporeSigma in the US and Canada



b) Color	white
c) Odor	weak
d) Melting point/freezing point	Melting point: 230 °C
e) Initial boiling point and boiling range	No data available
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	244 °C - closed cup
i) Autoignition temperature	210 °C at 0,3 hPa
j) Decomposition temperature	No data available
k) pH	5,0 - 7 at 36,4 g/l at 25 °C
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	36,4 g/l at 20 °C - completely soluble
n) Partition coefficient: n-octanol/water	log Pow: 2,26 - (Lit.), Bioaccumulation is not expected.
o) Vapor pressure	No data available
p) Density	2,30 g/cm <sup>3</sup>
Relative density	No data available
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

## 9.2 Other safety information

Bulk density	ca.390 kg/m <sup>3</sup>
Surface tension	39 mN/m at 25 °C

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## 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.



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

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## **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

Inhalation: No data available

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: Aqueous solution

#### **Germ cell mutagenicity**

No data available



**Carcinogenicity**

No data available

**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****Endocrine disrupting properties****Product:**

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Repeated dose toxicity - Rabbit - male and female - Dermal - 28 d - LOAEL (Lowest observed adverse effect level) - 10 mg/kg

Remarks: (in analogy to similar products)

Repeated dose toxicity - Rat - male and female - Oral - 28 d - NOAEL (No observed adverse effect level) - 100 mg/kg

Remarks: (as aqueous solution)  
(ECHA)

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

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**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 invertebrates	semi-static test EC50 - Daphnia magna (Water flea) - 0,037 mg/l - 48 h (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)





Toxicity to bacteria EC50 - activated sludge - 19 mg/l  
Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) NOEC - Daphnia magna (Water flea) - 0,023 mg/l - 21 d (OECD Test Guideline 211)

### 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 Endocrine disrupting properties

#### Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

### 12.7 Other adverse effects

Very toxic to aquatic life.

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### **Product**

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## 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-





**Full text of other abbreviations**

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

**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](http://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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