

**SAFETY DATA SHEET**

according to Regulation (EC) No. 1907/2006

Revision Date 12.09.2018

Version 12.4

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**SECTION 1. Identification of the substance/mixture and of the company/undertaking****1.1 Product identifier**

Catalogue No. 814119

Product name Hexadecyltrimethylammonium bromide for synthesis

REACH Registration Number A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. 57-09-0

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

Identified uses Chemical for synthesis  
For additional information on uses please refer to the Merck Chemicals portal ([www.merckgroup.com](http://www.merckgroup.com)).

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

Company Merck KGaA \* 64271 Darmstadt \* Germany \* Phone:+49 6151 72-0

Responsible Department LS-QHC \* e-mail: [prodsafe@merckgroup.com](mailto:prodsafe@merckgroup.com)

**1.4 Emergency telephone number** Please contact the regional company representation in your country.

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**SECTION 2. Hazards identification****2.1 Classification of the substance or mixture**

Classification (REGULATION (EC) No 1272/2008)

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Acute toxicity, Category 4, Oral, 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, Category 2, Oral, Gastrointestinal tract, H373

Acute aquatic toxicity, Category 1, H400

Chronic aquatic toxicity, Category 1, H410

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

## 2.2 Label elements

### Labelling (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 (Gastrointestinal tract) through prolonged or repeated exposure if swallowed.

H410 Very toxic to aquatic life with long lasting effects.

#### *Precautionary statements*

Prevention

P273 Avoid release to the environment.

P280 Wear eye protection.

Response

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

## Reduced labelling (≤125 ml)

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H318 Causes serious eye damage.

*Precautionary statements*

P280 Wear eye protection.

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

Contains: N-Cetyl-N'N'N-trimethylammonium bromide

CAS-No. 57-09-0

## 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula	$C_{16}H_{33}N(CH_3)_3Br$	$C_{19}H_{42}BrN$ (Hill)
EC-No.	200-311-3	
Molar mass	364,45 g/mol	

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## Hazardous components (REGULATION (EC) No 1272/2008)

*Chemical name (Concentration)*

CAS-No.	Registration number	Classification
N-Cetyl-N'N'N-trimethylammonium bromide (<= 100 % )		
57-09-0	*)	

Acute toxicity, Category 4, H302

Skin irritation, Category 2, H315

Serious eye damage, Category 1, H318

Specific target organ toxicity - single exposure, Category 3, H335

Specific target organ toxicity - repeated exposure, Category 2,  
H373

Acute aquatic toxicity, Category 1, H400

Chronic aquatic toxicity, Category 1, H410

M-Factor: 100

\*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

### 3.2 Mixture

Not applicable

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## SECTION 4. First aid measures

### 4.1 Description of first aid measures

After inhalation: fresh air. Call in physician.

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

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

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

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Breathing difficulties, depressed respiration, agitation, cardiovascular disorders, Convulsions  
Irritation and corrosion, Cough, Shortness of breath  
Risk of serious damage to eyes.

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

No information available.

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## SECTION 5. Firefighting measures

### 5.1 Extinguishing media

*Suitable extinguishing media*

Water, Foam, Carbon dioxide (CO<sub>2</sub>), Dry powder

*Unsuitable extinguishing media*

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

### 5.2 Special hazards arising from the substance or mixture

Combustible.

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

Fire may cause evolution of:

hydrogen bromide, nitrogen oxides

### 5.3 Advice for firefighters

*Special protective equipment 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.

*Further information*

Suppress (knock down) gases/vapours/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.

Advice for emergency responders:

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Protective equipment 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

Indications about waste treatment see section 13.

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## SECTION 7. Handling and storage

### 7.1 Precautions for safe handling

#### *Advice on safe handling*

Observe label precautions.

#### *Hygiene measures*

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

### 7.2 Conditions for safe storage, including any incompatibilities

#### *Storage conditions*

Tightly closed. Dry.

Recommended storage temperature see product label.

### 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

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## Derived No Effect Level (DNEL)

Worker DNEL, acute	Local effects	inhalation	0,05 mg/m <sup>3</sup>
Worker DNEL, longterm	Systemic effects	dermal	0,4 mg/kg Body weight
Worker DNEL, longterm	Local effects	dermal	0,05 mg/cm <sup>2</sup>
Worker DNEL, acute	Local effects	dermal	0,25 mg/cm <sup>2</sup>

## Predicted No Effect Concentration (PNEC)

PNEC Fresh water	0,022 µg/l
PNEC Marine water	0,0022 µg/l
PNEC Aquatic intermittent release	0,4 µg/l
PNEC Sewage treatment plant	0,19 mg/l
PNEC Soil	0,21 mg/kg

## 8.2 Exposure controls

### Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

### Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

#### *Eye/face protection*

Tightly fitting safety goggles

#### *Hand protection*

full contact:

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Glove material: Nitrile rubber  
Glove thickness: 0,11 mm  
Break through time: > 480 min

splash contact:

Glove material: Nitrile rubber  
Glove thickness: 0,11 mm  
Break through time: > 480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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)).

### *Other protective equipment*

protective clothing

### *Respiratory protection*

required when dusts are generated.

Recommended Filter type: Filter P 2 (acc. to DIN 3181) for solid and liquid particles of harmful substances

The entrepreneur 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.

### **Environmental exposure controls**

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**

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Form	solid
Colour	white
Odour	weak
Odour Threshold	No information available.
pH	5 - 7 at 50 g/l 20 °C
Melting point	237 - 243 °C
Boiling point	No information available.
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	No information available.
Relative vapour density	No information available.
Density	No information available.
Relative density	No information available.

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Water solubility	55 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 2,26 (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	> 230 °C
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

## 9.2 Other data

Bulk density	ca.390 kg/m <sup>3</sup>
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## SECTION 10. Stability and reactivity

### 10.1 Reactivity

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

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no information available

## 10.5 Incompatible materials

no information 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 oral toxicity*

LD50 Rat: 410 mg/kg

(RTECS)

#### *Acute inhalation toxicity*

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:., damage of respiratory tract

#### *Acute dermal toxicity*

This information is not available.

#### *Skin irritation*

Causes skin irritation.

#### *Eye irritation*

Causes serious eye damage.

#### *Sensitisation*

Result: Based on available data the classification criteria are not met.

#### *Germ cell mutagenicity*

This information is not available.

#### *Carcinogenicity*

This information is not available.

#### *Reproductive toxicity*

This information is not available.

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## *Teratogenicity*

This information is not available.

## *Specific target organ toxicity - single exposure*

May cause respiratory irritation.

Target Organs: Respiratory system

## *Specific target organ toxicity - repeated exposure*

May cause damage to organs through prolonged or repeated exposure.

Exposure routes: Ingestion

Target Organs: Gastrointestinal tract

## *Aspiration hazard*

This information is not available.

## **11.2 Further information**

After absorption:

agitation, depressed respiration, Convulsions, Shortness of breath, cardiovascular disorders

Under given conditions, contact with nitrites or nitric acid can lead to the formation of nitrosamines, which have shown themselves to be carcinogenic in animal experiments.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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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

Analytical monitoring: yes

OECD Test Guideline 203

#### *Toxicity to daphnia and other aquatic invertebrates*

Immobilization EC50 Daphnia magna (Water flea): 0,037 mg/l; 48 h

Analytical monitoring: yes

OECD Test Guideline 202

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## *Toxicity to algae*

Growth rate NOEC *Desmodesmus subspicatus* (green algae): 0,001 mg/l; 72 h  
(ECHA)

static test EC50 *Pseudokirchneriella subcapitata* (green algae): 0,00411 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

## *Toxicity to bacteria*

EC50 *Photobacterium phosphoreum*: 9,8 mg/l; 5 min

(Lit.)

## *Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)*

NOEC *Daphnia* (water flea): 0,023 mg/l; 21 d

OECD Test Guideline 211

## **12.2 Persistence and degradability**

### *Biodegradability*

100 %; 11 d; aerobic Chemical oxygen demand

OECD Test Guideline 301E

Readily biodegradable

> 95 %; 48 h

OECD Test Guideline 302B

Readily eliminated from water

## **12.3 Bioaccumulative potential**

*Partition coefficient: n-octanol/water*

log Pow: 2,26

(Lit.) Bioaccumulation is not expected.

## **12.4 Mobility in soil**

No information available.

## **12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

## **12.6 Other adverse effects**

Discharge into the environment must be avoided.

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## SECTION 13. Disposal considerations

### *Waste treatment methods*

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

### Land transport (ADR/RID)

14.1 UN number UN 3077  
14.2 Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (HEXADECYLTRIMETHYLAMMONIUMBROMIDE)  
14.3 Class 9  
14.4 Packing group III  
14.5 Environmentally hazardous yes  
14.6 Special precautions for user yes  
Tunnel restriction code -  
Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

### Inland waterway transport (ADN)

Not relevant

### Air transport (IATA)

14.1 UN number UN 3077  
14.2 Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (HEXADECYLTRIMETHYLAMMONIUMBROMIDE)  
14.3 Class 9  
14.4 Packing group III  
14.5 Environmentally hazardous yes

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**14.6 Special precautions for user** no

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

## Sea transport (IMDG)

**14.1 UN number** UN 3077

**14.2 Proper shipping name** ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID,  
N.O.S. (HEXADECYLTRIMETHYLAMMONIUMBROMIDE)

**14.3 Class** 9

**14.4 Packing group** III

**14.5 Environmentally hazardous** yes

**14.6 Special precautions for user** yes

EmS F-A S-F

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

**14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code**

Not relevant

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## SECTION 15. Regulatory information

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

#### *EU regulations*

Major Accident Hazard SEVESO III  
Legislation ENVIRONMENTAL HAZARDS  
E1  
Quantity 1: 100 t  
Quantity 2: 200 t

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Substances of very high concern (SVHC) This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of  $\geq 0.1$  % (w/w).

#### *National legislation*

Storage class 10 - 13

## 15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out.

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## 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.

### Training advice

Provide adequate information, instruction and training for operators.

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## Labelling

### *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 (Gastrointestinal tract) through prolonged or repeated exposure if swallowed.

H410 Very toxic to aquatic life with long lasting effects.

### *Precautionary statements*

#### Prevention

P273 Avoid release to the environment.

P280 Wear eye protection.

#### Response

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

Contains: N-Cetyl-N'N'N-trimethylammonium bromide

## Key or legend to abbreviations and acronyms used in the safety data sheet

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Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

## **Regional representation**

This information is given on the authorised Safety Data Sheet for your country.

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*The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.*