



# MATERIAL SAFETY DATA SHEET

according to the Hazard Communication Standard (29 CFR 1910.1200)

Date of issue: 07/05/2012

Version 1.0

## SECTION 1. Identification

### Product identifier

Product number	814119
Product name	Hexadecyltrimethylammonium bromide for synthesis

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

Identified uses	Chemical for synthesis
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### Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation   290 Concord Road, Billerica, MA 01821, United States of America   SDS Phone Support: +1-978-715-1335   General Inquiries: +1-978-715-4321   Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)  e-mail: mm_sds@merckgroup.com
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Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
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## SECTION 2. Hazards identification

### GHS Classification

Acute toxicity, Category 4, Oral, H302  
Specific target organ systemic toxicity - single exposure, Category 3, H335  
Skin irritation, Category 2, H315  
Eye irritation, Category 2, H319  
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.

### GHS-Labeling

#### Hazard pictograms



Signal Word  
Warning

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## *Hazard Statements*

H302 Harmful if swallowed.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

H410 Very toxic to aquatic life with long lasting effects.

## *Precautionary Statements*

P273 Avoid release to the environment.

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

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position 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.

## **OSHA Hazards**

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

## **Other hazards**

None known.

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## **SECTION 3. Composition/information on ingredients**

Formula	$C_{16}H_{33}N(CH_3)_3Br$	$C_{19}H_{42}BrN$ (Hill)
CAS-No.	57-09-0	
Molar mass	364.45 g/mol	

## **Hazardous ingredients**

*Chemical Name ( Concentration)*

CAS-No.

*N-Cetyl-N,N,N-trimethylammonium bromide ( <= 100 % )*

57-09-0

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## **SECTION 4. First aid measures**

### **Description of first-aid measures**

#### *Inhalation*

After inhalation: fresh air. Consult doctor if feeling unwell.

#### *Skin contact*

After skin contact: wash off with plenty of water. Remove contaminated clothing.

#### *Eye contact*

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

#### *Ingestion*

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

Never give anything by mouth to an unconscious person.

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### Most important symptoms and effects, both acute and delayed

Irritation and corrosion, irritant effects, Cough, Breathing difficulties, depressed respiration, Shortness of breath, agitation, cardiovascular disorders, Convulsions

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

No information available.

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## SECTION 5. Fire-fighting measures

### Extinguishing media

*Suitable extinguishing media*

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

*Unsuitable extinguishing media*

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

### Special hazards arising from the substance or mixture

Combustible material

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

Fire may cause evolution of:

hydrogen bromide, nitrogen oxides

### Advice for firefighters

*Special protective equipment for fire-fighters*

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/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

### 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: Protective equipment see section 8.

### Environmental precautions

Do not empty into drains.

### 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.

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## SECTION 7. Handling and storage

### Precautions for safe handling

Observe label precautions.

### Conditions for safe storage, including any incompatibilities

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Tightly closed. Dry.

Store at +15°C to +25°C (+59°F to +77°F).

## SECTION 8. Exposure controls/personal protection

### Exposure limit(s)

Contains no substances with occupational exposure limit values.

### Engineering measures

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

### Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

### Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

### Eye/face protection

Safety glasses

### Hand protection

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Recommended:

full contact:

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

### Other protective equipment:

protective clothing

### Respiratory protection

required when dusts are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

## SECTION 9. Physical and chemical properties

Physical state

solid

Color

white

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Odor	weak
Odor Threshold	No information available.
pH	5 - 7 at 50 g/l 68 °F ( 20 °C)
Melting point	459 - 469 °F ( 237 - 243 °C)
Boiling point	No information available.
Flash point	not applicable
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapor pressure	No information available.
Relative vapor density	No information available.
Relative density	No information available.
Water solubility	3 g/l at 68 °F ( 20 °C)
Partition coefficient: n-octanol/water	log Pow: 2.26 (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	> 446 °F ( > 230 °C)
Viscosity, dynamic	No information available.
Bulk density	ca. 390 kg/m <sup>3</sup>

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### SECTION 10. Stability and reactivity

#### Reactivity

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

#### Chemical stability

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

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### Possibility of hazardous reactions

Strong oxidizing agents

Violent reactions possible with:

### Conditions to avoid

Heating.

### Incompatible materials

no information available

### Hazardous decomposition products

in the event of fire: See section 5.

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## SECTION 11. Toxicological information

### Information on toxicological effects

#### *Likely route of exposure*

Eye contact, Skin contact, Ingestion

#### *Acute oral toxicity*

LD50 rat: 410 mg/kg (RTECS)

Symptoms: Convulsions, Breathing difficulties, cardiovascular disorders  
absorption

#### *Acute inhalation toxicity*

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

Irritating to respiratory system.

#### *Skin irritation*

Irritations

Causes skin irritation.

#### *Eye irritation*

rabbit

Result: Severe irritations

Causes serious eye irritation.

#### *Specific target organ systemic toxicity - single exposure*

May cause respiratory irritation.

#### *Specific target organ systemic toxicity - repeated exposure*

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

#### *Aspiration hazard*

Regarding the available data the classification criteria are not fulfilled.

### Carcinogenicity

IARC

No ingredient of this product present at levels greater than or  
equal to 0.1% is identified as probable, possible or confirmed

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	human carcinogen by IARC.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

### Further information

Systemic effects:

If swallowed

agitation, depressed respiration

Further data:

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

### Ecotoxicity

*Toxicity to fish*

LC50 Danio rerio (zebra fish): 0.3 mg/l; 96 h (External MSDS)

*Toxicity to daphnia and other aquatic invertebrates*

EC50 Daphnia magna (Water flea): 0.22 mg/l; 24 h (Lit.)

*Toxicity to algae*

IC50 M.aeruginosa: 0.03 mg/l; 96 h (Lit.)

IC50 Desmodesmus subspicatus (green algae): 0.01 mg/l; 72 h (Lit.)

*Toxicity to bacteria*

EC50 Photobacterium phosphoreum: 9.8 mg/l; 5 min (Lit.)

### Persistence and degradability

*Biodegradability*

74 %; 28 d

OECD Test Guideline 301E

Not readily biodegradable.

> 95 %; 48 h

OECD Test Guideline 302B

Readily eliminated from water

### Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: 2.26

(Lit.) Bioaccumulation is not expected (log Pow <1).

### Mobility in soil

No information available.

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## Other adverse effects

*Stability in water*

4 - 9 d

(Lit.) Rapid degradation.

*Additional ecological information*

Discharge into the environment must be avoided.

## SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

## SECTION 14. Transport information

### Land transport (DOT)

UN number

UN 3077

Proper shipping name

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID,  
N.O.S. ( HEXADECYLTRIMETHYLAMMONIUMBROMIDE)

Class

9

Packing group

III

Environmentally hazardous

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### Air transport (IATA)

UN number

UN 3077

Proper shipping name

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID,  
N.O.S. ( HEXADECYLTRIMETHYLAMMONIUMBROMIDE)

Class

9

Packing group

III

Environmentally hazardous

--

Special precautions for user

no

### Sea transport (IMDG)

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UN number	UN 3077
Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. ( HEXADECYLTRIMETHYLAMMONIUMBROMIDE)
Class	9
Packing group	III
Environmentally hazardous	--
Special precautions for user	yes
EmS	F-A S-F

## SECTION 15. Regulatory information

### United States of America

#### OSHA Hazards

Toxic by ingestion

Skin irritant

Eye irritant

Respiratory irritant

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

#### SARA 311/312 Hazards

Acute Health Hazard

### US State Regulations

#### Massachusetts Right To Know

Remarks

No components are subject to the Massachusetts Right to Know Act.

#### Pennsylvania Right To Know

*Ingredients*

N-Cetyl-N'N'N-trimethylammonium bromide

#### New Jersey Right To Know

*Ingredients*

N-Cetyl-N'N'N-trimethylammonium bromide

#### California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

#### Notification status

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TSCA:

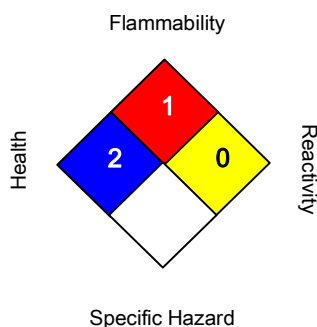
On TSCA Inventory

DSL:

All components of this product are on the Canadian DSL list.

## SECTION 16. Other information

### National Fire Protection Association (U.S.A)



### Training advice

Provide adequate information, instruction and training for operators.

### Full text of H-Statements referred to under sections 2 and 3.

H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

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

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

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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