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

1.1 Product identifiers

Product name: Hexadecyltrimethylammonium bromide

Product Number: H9151
Brand: Sigma
REACH No.: A registration number is not available for this substance as the substance or its uses are exempted from registration, 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: Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Chemie BV
Stationsplein 4
3331 LL ZWIJNDRECHT
NETHERLANDS

Telephone: +31 78-620-5411
Fax: +31 78-620-5421
E-mail address: eurtechserv@sial.com

1.4 Emergency telephone number

Emergency Phone #: 112

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
Acute aquatic toxicity (Category 1), H400

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

Classification according to EU Directives 67/548/EEC or 1999/45/EC
Xn, N Harmful, Dangerous for the R22, R37/38, R41, R50, R48/22 environment

For the full text of the R-phrases mentioned in this Section, see Section 16.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008
Pictogram

SIGMA-ALDRICH

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006
Version 5.7 Revision Date 14.01.2015
Print Date 19.03.2015

GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA
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.
H400  Very toxic to aquatic life.

Precautionary statement(s):

P261  Avoid breathing dust.
P273  Avoid release to the environment.
P280  Wear protective gloves/ eye protection/ face 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.

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
- Palmitryltrimethylammonium bromide
- CTAB
- Cetyltrimethylammonium bromide

Formula: \(C_{19}H_{42}BrN\)
Molecular weight: 364.45 g/mol
CAS-No.: 57-09-0
EC-No.: 200-311-3

Hazardous ingredients according to Regulation (EC) No 1272/2008

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cetrimonium bromide</td>
<td>Acute Tox. 4; Skin Irrit. 2; Eye Dam. 1; STOT SE 3; STOT RE 2; Aquatic Acute 1; H302, H315, H318, H335, H373, H400</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
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<tbody>
<tr>
<td>Cetrimonium bromide</td>
<td>Xn, N, R22 - R37/38 - R41 - R48/22 - R50</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

Hazardous ingredients according to Directive 1999/45/EC

For the full text of the H-Statements and R-Phrases mentioned in this Section, see Section 16

SECTION 4: First aid measures

4.1 Description of first aid measures

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance.
If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
Never give anything by mouth to an unconscious person. Rinse mouth with water. 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 (NOx), Hydrogen bromide gas

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
No data available

SECTION 6: Accidental release measures
6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage
7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Storage class (TRGS 510): Non Combustible Solids

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated
SECTION 8: Exposure controls/personal protection

8.1 Control parameters
Components with workplace control parameters

8.2 Exposure controls
Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0,11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0,11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

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
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: solid

b) Odour
   No data available

c) Odour Threshold
   No data available

d) pH
   5.0 - 7 at 36.4 g/l at 25 °C

e) Melting point/freezing point
   Melting point/range: 248 - 251 °C

f) Initial boiling point and boiling range
   No data available

g) Flash point
   244 °C - closed cup

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

j) Upper/lower flammability or explosive limits
   No data available

k) Vapour pressure
   No data available

l) Vapour density
   No data available

m) Relative density
   No data available

n) Water solubility
   36.4 g/l at 20 °C - completely soluble

o) Partition coefficient: n-octanol/water
   log Pow: 3.18

p) Auto-ignition temperature
   No data available

q) Decomposition temperature
   No data available

r) Viscosity
   No data available

s) Explosive properties
   No data available

t) Oxidizing properties
   No data available

9.2 Other safety information
   No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
   No data available

10.2 Chemical stability
   Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
   No data available

10.4 Conditions to avoid
   No data available

10.5 Incompatible materials
   Strong oxidizing agents

10.6 Hazardous decomposition products
   Other decomposition products - No data available
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

**Acute toxicity**
LD50 Oral - Rat - 410 mg/kg

**Skin corrosion/irritation**
Skin - Rabbit
Result: Moderate skin irritation

**Serious eye damage/eye irritation**
Eyes - Rabbit
Result: Severe eye irritation

**Respiratory or skin sensitisation**
No data available

**Germ cell mutagenicity**
No data available

**Carcinogenicity**
IARC: No component 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.

**Specific target organ toxicity - repeated exposure**
Oral - May cause damage to organs through prolonged or repeated exposure. - Gastrointestinal tract

**Aspiration hazard**
No data available

**Additional Information**
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
LC50 - Danio rerio (zebra fish) - 0,3 mg/l - 96,0 h

Toxicity to daphnia and other aquatic invertebrates
EC50 - Daphnia magna (Water flea) - 0,03 mg/l - 48 h

12.2 Persistence and degradability
Biodegradability Result: - Biodegradable

12.3 Bioaccumulative potential
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.
Very toxic to aquatic life.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging
Dispose of as unused product.

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. (Cetrimonium bromide)  
(Cetrimonium bromide)  
IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Cetrimonium bromide)  
(Cetrimonium bromide)  
IATA: Environmentally hazardous substance, solid, n.o.s. (Cetrimonium bromide) (Cetrimonium 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

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.

SECTION 15: Regulatory information

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

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

No data available

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.

Acute Tox. Acute toxicity
Aquatic Acute Acute aquatic toxicity
Eye Dam. Serious eye damage
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.
Skin Irrit. Skin irritation
STOT RE Specific target organ toxicity - repeated exposure
STOT SE Specific target organ toxicity - single exposure

**Full text of R-phrases referred to under sections 2 and 3**

N Dangerous for the environment
Xn Harmful
R22 Harmful if swallowed.
R37/38 Irritating to respiratory system and skin.
R41 Risk of serious damage to eyes.
R48/22 Harmful: danger of serious damage to health by prolonged exposure if swallowed.
R50 Very toxic to aquatic organisms.

**Further information**

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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.