

## Material Safety Data Sheet

Date Printed: 30/JUL/2007

Date Updated: 05/MAR/2007

Version 1.10

Regulation (EC) No 1907/2006

## 1 - Product and Company Information

Product Name	HEXADECYLTRIMETHYLAMMONIUM BROMIDE
Product Number	H5882
Company	Sigma-Aldrich Pte Ltd #02-14 The Capricorn, Sci. Park II Singapore 117528 Singapore
Technical Phone #	(65) 6779 1200
Fax	(65) 6779 1822

## 2 - Hazards Identification

## SPECIAL INDICATION OF HAZARDS TO HUMANS AND THE ENVIRONMENT

Harmful if swallowed. Irritating to respiratory system and skin.

Risk of serious damage to eyes. Very toxic to aquatic organisms.

## 3 - Composition/Information on Ingredients

Product Name	CAS #	EC no	Annex I Index Number
CETYLTRIMETHYL AMMONIUM BROMIDE	57-09-0	200-311-3	None

Formula	C19H42N.Br
Molecular Weight	364.46 AMU
Synonyms	Acetoquat CTAB * Bromat * Centimide * Cetarol * Cetrimonium bromide * Cetyltrimethylammonium bromide * N-Cetyltrimethylammonium bromide * Cirrasol-OD * CTAB * Cycloton V * 1-Hexadecanaminium, N,N,N-trimethyl-, bromide * Hexadecyltrimethylammonium bromide * N-Hexadecyl-N,N,N-trimethylammonium bromide * (1-Hexadecyl)trimethylammonium bromide * Lauroseptol * Lissolamine * Lissolamine A * Micol * Palmityltrimethyl ammonium bromide * Pollacid * Quamonium * Softex KW * Trimethylcetylammmonium bromide * N,N,N-Trimethyl-1-hexadecanaminium bromide * Trimethylhexadecylammmonium bromide

## 4 - First Aid Measures

## AFTER INHALATION

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

## AFTER SKIN CONTACT

In case of contact, immediately wash skin with soap and copious amounts of water.

## AFTER EYE CONTACT

In case of contact, immediately flush eyes with copious amounts of water for at least 15 minutes.

#### AFTER INGESTION

If swallowed, wash out mouth with water provided person is conscious. Call a physician.

---

### 5 - Fire Fighting Measures

---

#### EXTINGUISHING MEDIA

Suitable: Water spray. Carbon dioxide, dry chemical powder, or appropriate foam.

#### SPECIAL RISKS

Specific Hazard(s): Emits toxic fumes under fire conditions.

#### SPECIAL PROTECTIVE EQUIPMENT FOR FIREFIGHTERS

Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.

---

### 6 - Accidental Release Measures

---

#### PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear respirator, chemical safety goggles, rubber boots, and heavy rubber gloves.

#### METHODS FOR CLEANING UP

Sweep up, place in a bag and hold for waste disposal. Avoid raising dust. Ventilate area and wash spill site after material pickup is complete.

---

### 7 - Handling and Storage

---

#### HANDLING

Directions for Safe Handling: Do not breathe dust. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

#### STORAGE

Conditions of Storage: Keep tightly closed.

---

### 8 - Exposure Controls / Personal Protection

---

#### ENGINEERING CONTROLS

Safety shower and eye bath. Mechanical exhaust required.

#### GENERAL HYGIENE MEASURES

Wash thoroughly after handling.

#### PERSONAL PROTECTIVE EQUIPMENT

Respiratory Protection: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a dust mask type N95 (US) or type P1 (EN 143) respirator.

Hand Protection: Compatible chemical-resistant gloves.

Eye Protection: Chemical safety goggles.

---

### 9 - Physical and Chemical Properties

---

Appearance

Physical State: Solid

Property	Value	At Temperature or Pressure
pH	5.0 - 7.0	
BP/BP Range	N/A	
MP/MP Range	230 °C	
Flash Point	244 °C	Method: closed cup
Flammability	N/A	
Autoignition Temp	N/A	
Oxidizing Properties	N/A	
Explosive Properties	N/A	
Explosion Limits	N/A	
Vapor Pressure	N/A	
SG/Density	N/A	
Partition Coefficient	Log Kow: 3.18	
Viscosity	N/A	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
Evaporation Rate	N/A	
Bulk Density	N/A	
Decomposition Temp.	N/A	
Solvent Content	N/A	
Water Content	N/A	
Surface Tension	N/A	
Conductivity	N/A	
Miscellaneous Data	N/A	
Solubility	Solubility in Water: 0.1 M in H <sub>2</sub> O, 20°C complete, colorless	

---

## 10 - Stability and Reactivity

---

### STABILITY

Stable: Stable.

Materials to Avoid: Strong oxidizing agents.

### HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide, Nitrogen oxides, Hydrogen bromide gas.

### HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

---

## 11 - Toxicological Information

---

RTECS NUMBER: BQ7875000

### ACUTE TOXICITY

LD50  
Oral  
Rat  
410 mg/kg

LD50  
Intravenous  
Rat  
44 MG/KG  
Remarks: Lungs, Thorax, or Respiration: Other changes.

LD50  
Intraperitoneal  
Mouse  
106 MG/KG

Remarks: Behavioral:Convulsions or effect on seizure threshold.  
Lungs, Thorax, or Respiration:Respiratory depression.

LD50

Intravenous

Mouse

32 MG/KG

Remarks: Lungs, Thorax, or Respiration:Other changes.

LD50

Intraperitoneal

Rabbit

125 MG/KG

LD50

Subcutaneous

Rabbit

125 MG/KG

LD50

Subcutaneous

Guinea pig

100 MG/KG

#### IRRITATION DATA

Skin

Mouse

50 mg

1H

Remarks: Open irritation test

Eyes

Rabbit

450 mg

Remarks: Severe irritation effect

#### SIGNS AND SYMPTOMS OF EXPOSURE

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

#### ROUTE OF EXPOSURE

Skin Contact: Causes skin irritation.

Skin Absorption: May be harmful if absorbed through the skin.

Eye Contact: Causes severe eye irritation.

Inhalation: May be harmful if inhaled. Material is irritating to mucous membranes and upper respiratory tract.

Ingestion: Harmful if swallowed.

#### CHRONIC EXPOSURE - TERATOGEN

Species: Mouse

Dose: 10500 UG/KG

Route of Application: Intraperitoneal

Exposure Time: (8D PREG)

Result: Specific Developmental Abnormalities: Musculoskeletal system.

Species: Mouse

Dose: 10500 UG/KG

Route of Application: Intraperitoneal

Exposure Time: (10D PREG)

Result: Specific Developmental Abnormalities: Craniofacial (including nose and tongue).

Species: Mouse

Dose: 35 MG/KG

Route of Application: Intraperitoneal

Exposure Time: (12D PREG)

Result: Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

#### CHRONIC EXPOSURE - REPRODUCTIVE HAZARD

Species: Mouse

Dose: 35 MG/KG

Route of Application: Intraperitoneal

Exposure Time: (8D PREG)

Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).

---

#### 12 - Ecological Information

---

##### ELIMINATION

Elimination: 100 %

##### ECOTOXICOLOGICAL EFFECTS

Test Type: EC50 Daphnia

Species: Daphnia magna

Time: 48 h

Value: 0.03 mg/l

Test Type: LC50 Fish

Species: Brachydanio rerio

Time: 96 h

Value: 0.3 mg/l

---

#### 13 - Disposal Considerations

---

##### SUBSTANCE DISPOSAL

Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

---

#### 14 - Transport Information

---

##### RID/ADR

UN#: 3077

Class: 9

PG: III

Proper Shipping Name: Environmentally hazardous substance, solid, n.o.s

##### IMDG

UN#: 3077

Class: 9

PG: III

Proper Shipping Name: Environmentally hazardous substance, solid, n.o.s

Marine Pollutant: No

Severe Marine Pollutant: No

Technical Name: Required

IATA

UN#: 3077

Class: 9

PG: III

Proper Shipping Name: Environmentally hazardous  
substance, solid, n.o.s

Inhalation Packing Group I: No

Technical Name: Required

---

15 - Regulatory Information

---

CLASSIFICATION AND LABELING ACCORDING TO EU DIRECTIVES

INDICATION OF DANGER: Xn-N

Harmful. Dangerous for the environment.

R-PHRASES: 22-37/38-41-50

Harmful if swallowed. Irritating to respiratory system and  
skin. Risk of serious damage to eyes. Very toxic to aquatic  
organisms.

S-PHRASES: 26-39-61

In case of contact with eyes, rinse immediately with plenty of  
water and seek medical advice. Wear eye/face protection. Avoid  
release to the environment. Refer to special  
instructions/safety data sheets.

COUNTRY SPECIFIC INFORMATION

Germany

WGK: 3

ID-Number: 600

KBwS-Decision

---

16 - Other Information

---

WARRANTY

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 Inc.,  
shall not be held liable for any damage resulting from handling or  
from contact with the above product. See reverse side of invoice  
or packing slip for additional terms and conditions of sale.  
Copyright 2007 Sigma-Aldrich Co. License granted to make unlimited  
paper copies for internal use only.

DISCLAIMER

For R&D use only. Not for drug, household or other uses.