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

1.1 Product identifiers

Product name: Benzethonium chloride

Product Number: 53751
Brand: Sigma
CAS-No.: 121-54-0

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

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO  63103
UNITED STATES

Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 3), H301
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
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 GHS Label elements, including precautionary statements

Pictogram

Sigma - 53751
Signal Word: Danger

Hazard statement(s):

H301  Toxic if swallowed.
H314  Causes severe skin burns and eye damage.
H410  Very toxic to aquatic life with long lasting effects.

Precautionary statement(s):

P260  Do not breathe dust.
P264  Wash skin thoroughly after handling.
P270  Do not eat, drink or smoke when using this product.
P273  Avoid release to the environment.
P280  Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310 + P330  IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P301 + P330 + P331  IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353  IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310  IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310  IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P363  Wash contaminated clothing before reuse.
P391  Collect spillage.
P405  Store locked up.
P501  Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms: Phemerol chloride

Formula: C_{27}H_{42}ClNO_2
Molecular weight: 448.08 g/mol
CAS-No.: 121-54-0
EC-No.: 204-479-9

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>benzethonium chloride</td>
<td>Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Aquatic Acute 1; Aquatic Chronic 1; H301, H314, H318, H400, H410 M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

Sigma - 53751
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
First aiders need to protect themselves. 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. Call a physician immediately.

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

If swallowed
If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible. Do not attempt to neutralise.

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
Water Foam Carbon dioxide (CO2) 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
Carbon oxides
Nitrogen oxides (NOx)
Hydrogen chloride gas
Combustible.
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.

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 carefully. Dispose of properly. Clean up affected area.
Avoid generation of dusts.

6.4 Reference to other sections
For disposal see section 13.

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. Keep in a well-ventilated place. Keep locked up or in an area accessible
only to qualified or authorized persons.
Light sensitive. hygroscopic Handle and store under inert gas.

Storage class
Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or
compounds which causing chronic effects

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
Ingredients with workplace control parameters
Contains no substances with occupational exposure limit values.
8.2 Exposure controls

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

**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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: 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

- **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**
Recommended Filter type: Filter type P3
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. Required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

**Control of environmental exposure**
Do not let product enter drains.
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: powder
   Color: white, off-white

b) Odor
   odorless

c) Odor Threshold
   Not applicable

d) pH
   5.5 - 7.5 at 44.8 g/l at 25 °C (77 °F)

e) Melting point/freezing point
   Melting point/range: 162 - 164 °C (324 - 327 °F) - lit.

f) Initial boiling point
   and boiling range
   >= 162 °C >= 324 °F - OECD Test Guideline 103

g) Flash point
   No data available

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

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

k) Vapor pressure
   < 0.001 hPa at 25 °C (77 °F) - OECD Test Guideline 104

l) Vapor density
   No data available

m) Density
   No data available
   Relative density
   1.120 °C - OECD Test Guideline 109

n) Water solubility
   44.8 g/l at 20 °C (68 °F)

o) Partition coefficient: n-octanol/water
   log Pow: 1.08 at 20 °C (68 °F) - OECD Test Guideline 107 - Bioaccumulation is not expected.

p) Autoignition temperature
   > 400 °C (> 752 °F) - Relative self-ignition temperature for solids does not ignite

q) Decomposition temperature
   162 - 164 °C (324 - 327 °F) - 

r) Viscosity
   No data available

s) Explosive properties
   No data available

t) Oxidizing properties
   none

9.2 Other safety information

Surface tension
   33.4 mN/m at 1g/l at 20 °C (68 °F) - OECD Test Guideline 115
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

10.4 Conditions to avoid
no information available

10.5 Incompatible materials
No data available

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - 295 mg/kg (US-EPA)
Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.
Inhalation: No data available
Dermal: No data available
Skin corrosion/irritation
Skin - Rabbit
Result: Causes burns. - 4 h (US-EPA)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Causes serious eye damage. - 24 h (OECD Test Guideline 405)
Remarks: Causes serious eye damage.

Respiratory or skin sensitization
Maximization Test - Guinea pig
Result: negative (OECD Test Guideline 406)

Germ cell mutagenicity
Test Type: Ames test
Test system: S. typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative

**Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

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.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA’s list of regulated carcinogens.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

RTECS: BO717500053752
burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Systemic effects:

Cyanosis
Convulsions
Coma

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

**SECTION 12: Ecological information**

**12.1 Toxicity**

Toxicity to fish semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - 1.15 mg/l - 96 h
(OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates

- static test EC50 - Daphnia magna (Water flea) - 0.22 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae

- static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 0.3 mg/l - 72 h (OECD Test Guideline 201)

Toxicity to bacteria

- EC50 - activated sludge - 35.7 mg/l - 3 h (OECD Test Guideline 209)

12.2 **Persistence and degradability**

Biodegradability

- aerobic - Exposure time 28 d
  - Result: 0 % - Not biodegradable (OECD Test Guideline 301B)

12.3 **Bioaccumulative potential**

- No data available

12.4 **Mobility in soil**

- No data available

12.5 **Results of PBT and vPvB assessment**

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

12.6 **Endocrine disrupting properties**

- No data available

12.7 **Other adverse effects**

- Discharge into the environment must be avoided.

---

**SECTION 13: Disposal considerations**

13.1 **Waste treatment methods**

**Product**

- Waste material must be disposed of in accordance with the national and local regulations.
- Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

---

**SECTION 14: Transport information**

**DOT (US)**

- UN number: 2923  
  - Class: 8 (6.1)  
  - Packing group: III  
  - Proper shipping name: Corrosive solids, toxic, n.o.s. (benzethonium chloride)  
  - Reportable Quantity (RQ):
    - Poison Inhalation Hazard: No

**IMDG**

- UN number: 2923  
  - Class: 8 (6.1)  
  - Packing group: III  
  - EMS-No: F-A, S-B  
  - Proper shipping name: CORROSIVE SOLID, TOXIC, N.O.S. (benzethonium chloride)  
  - Marine pollutant: yes
**SECTION 15: Regulatory information**

**IATA**
UN number: 2923     Class: 8 (6.1)     Packing group: III
Proper shipping name: Corrosive solid, toxic, n.o.s. (benzethonium chloride)

**SECTION 15: Regulatory information**

**SARA 302 Components**
This material does not contain any components with a section 302 EHS TPQ.

**SARA 313 Components**
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**
Acute Health Hazard

**Massachusetts Right To Know Components**
No components are subject to the Massachusetts Right to Know Act.

**SECTION 16: Other information**

**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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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