

Benzethonium Chloride SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Benzethonium Chloride

* Catalog Number: S4162

* CAS Number: 121-54-0

* IUPAC Name: Benzenemethanaminium, N,N-dimethyl-N-[2-[2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethoxy]ethyl]-, chloride (1:1)

Relevant identified uses and uses advised against

* Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.

* Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

* Company: Selleck Chemicals

* TollFree: +1 877 796-6397

* Tel: +1 832 582-8158

* Fax: +1 832 582-8590

Emergency telephone number

* Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

Acute toxicity (oral): Category 3. H301

Acute toxicity (oral): Category 4. H302

Skin corrosion: Category 1. H314

Skin irritation: Category 2. H315

Serious eye damage: Category 1. H318

Serious eye irritation: Category 2. H319

Acute aquatic toxicity: Category 1. H400

Chronic aquatic toxicity: Category 1. H410

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)	H301: Toxic if swallowed H302: Harmful if swallowed H314: Causes severe skin burns and eye damage H315: Causes skin irritation H318: Causes serious eye damage H319: Causes serious eye irritation H400: Very toxic to aquatic life H410: Very toxic to aquatic life with long lasting effects
Precautionary statement(s)	None.
Prevention	P260: Do not breathe dust/fume/gas/mist/vapors/spray. P264: Wash hands thoroughly after handling. P264+P265: Wash hands thoroughly after handling. Do not touch eyes. 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/hearing protection.
Response	P301+P316: IF SWALLOWED: Get emergency medical help immediately. P301+P317: IF SWALLOWED: Get medical help. P301+P330: IF SWALLOWED: Rinse mouth. P302+P352: IF ON SKIN: wash with plenty of water. P302+P361: IF ON SKIN: Take off immediately all contaminated clothing. P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing. P305+P351: IF IN EYES: Rinse cautiously with water for several minutes. P305+P354: IF IN EYES: Immediately rinse with water for several minutes. P316: Get emergency medical help immediately. P317: Get emergency medical help. P321: Specific treatment (see information on this label and safety datasheet)). P330: Rinse mouth. P331: Do NOT induce vomiting. P332+P317: If skin irritation occurs: Get medical help. P337+P317: If eye irritation persists: Get medical help. P338: Remove contact lenses, if present and easy to do. Continue rinsing. P354: Immediately rinse with water for several minutes. P362+P364: Take off contaminated clothing and wash it before reuse. P363: Wash contaminated clothing before reuse. P391: Collect spillage.
Storage	P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Benzethonium Chloride

CAS Number: 121-54-0

PubChem CID: 8478

Molecular formula: C₂₇H₄₂ClNO₂

Molecular weight: 448.1 g/mol

IUPAC name: benzyl-dimethyl-[2-[2-[4-(2,4,4-trimethylpentan-2-yl)phenoxy]ethoxy]ethyl]azanium chloride

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Fresh air, rest.

Skin contact: Remove contaminated clothes. Rinse and then wash skin with water and soap.

Eye contact: First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Ingestion: Rinse mouth. Give one or two glasses of water to drink. Refer for medical attention .

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO₂), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. (NTP, 1992)

Use water spray, powder.

Alcohol foam, carbon dioxide, dry chemical, water fog /Hyamine compd/

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

WARNING: Highly toxic — only trained personnel should handle spills.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

SMALL SPILLS AND LEAKAGE: If you spill this chemical, you should dampen the solid spill material with water, then transfer the dampened material to a suitable container. Use absorbent paper dampened with water to pick up any remaining material. Seal your contaminated clothing and the absorbent paper in a vapor-tight plastic bag for eventual disposal. Wash all contaminated surfaces with a soap and water solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned.

STORAGE PRECAUTIONS: You should protect this chemical from exposure to light. Keep the container tightly closed under an inert atmosphere, and store under refrigerated temperatures. (NTP, 1992)

Separated from food and feedstuffs. Store in an area without drain or sewer access. Dry.

... SOLUTIONS SHOULD BE STORED IN DISTINCTIVE BOTTLES (NEVER IN SOFT DRINK BOTTLES) IN A SAFE PLACE. /CATIONIC DETERGENTS/

IN GENERAL, MATERIALS WHICH ARE TOXIC AS STORED OR WHICH CAN DECOMP INTO TOXIC COMPONENTS ... SHOULD BE STORED IN A COOL, WELL-VENTILATED PLACE, OUT OF DIRECT RAYS OF THE SUN, AWAY FROM AREAS OF HIGH FIRE HAZARD, & SHOULD BE PERIODICALLY INSPECTED INCOMPATIBLE MATERIALS SHOULD BE ISOLATED FROM EACH OTHER.

7.2 Conditions for safe storage, including any incompatibilities

Separated from food and feedstuffs. Store in an area without drain or sewer access. Dry.

... SOLUTIONS SHOULD BE STORED IN DISTINCTIVE BOTTLES (NEVER IN SOFT DRINK BOTTLES) IN A SAFE PLACE. /CATIONIC DETERGENTS/

IN GENERAL, MATERIALS WHICH ARE TOXIC AS STORED OR WHICH CAN DECOMP INTO TOXIC COMPONENTS ... SHOULD BE STORED IN A COOL, WELL-VENTILATED PLACE, OUT OF DIRECT RAYS OF THE SUN, AWAY FROM AREAS OF HIGH FIRE HAZARD, & SHOULD BE PERIODICALLY INSPECTED INCOMPATIBLE MATERIALS SHOULD BE ISOLATED FROM EACH OTHER.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use in a well-ventilated area. Chemical fume hood recommended for powder handling.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear chemical safety goggles and face shield.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Respiratory protection usually not required under normal use with adequate ventilation.

Use N95 respirator for large-scale powder handling.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- a) Appearance: Benzethonium chloride appears as odorless white crystals or powder with a very bitter taste. A 1% solution in water is slightly alkaline to litmus. (NTP, 1992)
- b) Odor: MILD ODOR
- c) Odor threshold: No data available
- d) pH: PH OF 1% AQ SOLN IS BETWEEN 4.8 & 5.5
- e) Melting point/freezing point: 327 to 331 °F (NTP, 1992)
- f) Initial boiling point and boiling range: No data available
- 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: No data available
- l) Vapor density: No data available
- m) Relative density: No data available
- n) Water solubility: 10 to 50 mg/mL at 64 °F (NTP, 1992)
- o) Partition coefficient: n-octanol/water: Log P: No data available
- 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 information

Topological Polar Surface Area (TPSA): 18.5 Å²

Complexity: 466

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

Avoid strong oxidizing agents, strong acids, and strong bases.

10.5 Incompatible materials

INCOMPATIBILITIES: INCOMPATIBLE WITH & INACTIVATED BY SOAPS, ANIONIC DETERGENTS, ORGANIC MATERIAL, & NITRATES.

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Hydrogen chloride (HCl).

See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

No acute toxicity data available.

Skin corrosion/irritation:

Causes severe skin burns and eye damage (H314).

Serious eye damage/eye irritation:

Causes serious eye damage (H318).

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

No data available.

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

Carcinogen classification:

Benzethonium Chloride

TR-438: Toxicology and Carcinogenesis Studies of Benzethonium Chloride (CASRN 121-54-0) in F344/N Rats and B6C3F1 Mice (Dermal Studies) (1995)

06/21/94

No Evidence

No Evidence

No Evidence

No Evidence

Under the conditions of these 2-year dermal studies, there was no evidence of carcinogenic activity of benzethonium chloride in male or female F344/N rats receiving 0.15, 0.5, or 1.5 mg/kg. There was no evidence of carcinogenic activity in male or female B6C3F1 mice receiving

Exposure routes:

The substance can be absorbed into the body through the skin and by ingestion.

Signs and symptoms of exposure:

Redness. Pain.

Redness. Blurred vision. Pain. Severe burns.

Nausea. Vomiting. Diarrhoea. Convulsions. Shock or collapse.

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

LC50 Pimephales promelas 1600 ug/l/96 hr /Conditions of bioassay not specified/

LC50 Lepomis macrochirus 1400 ug/l/96 hr /Conditions of bioassay not specified/

LC50 Oncorhynchus kisutch 53000 ug/l/96 hr /Conditions of bioassay not specified/

The substance is toxic to aquatic organisms. It is strongly advised not to let the chemical enter into the environment.

CATIONIC SURFACTANTS HAD NOBACTERIOSTATIC OR BACTERIOLYTIC ACTION ON HETEROTROPHIC BACTERIAL POPULATION ISOLATED FROM SEWAGE & RIVER WATERS, CYCLICAL ALKYLAMMONIUM CMPD ARE NOT DEGRADED.

Biodegradation: at 18 mg/l no degradation after 28 days by nonadapted sewage.

12.2 Persistence and degradability

No data available.

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.

12.6 Other adverse effects

This substance is classified as hazardous to the aquatic environment.

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods**

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION**14.1 UN number**

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: Yes (classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

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

Not applicable.

15. REGULATORY INFORMATION**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Registered (REACH Active)

SARA 302 Components:

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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 (short-term) health hazard

Environmental hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

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

Other regulatory listings:

- The Australian Inventory of Industrial Chemicals: Chemical: Benzenemethanaminium, N,N-dimethyl-N-[2-[2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethoxy]ethyl]-, chloride
- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Hazard Trait Undefined Authoritative List - CECBP - Priority Chemicals Report - if used as a fragrance or flavor ingredient
- FDA Requirements: Manufacturers, packers, and distributors of drug and drug products for human use are responsible for complying with the labeling, certification, and usage requirements as prescribed by the Federal Food, Drug, and Cosmetic Act, as amended (secs 201-902, 52 Stat. 1040 et seq., as amended; 21 U.S.C. 32

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/09

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product. Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.