SAFETY DATA SHEET

Updated on 04/12/2024

1. Material Identification

Product Name : Benzethonium Chloride
Catalog Number : io-45023
CAS Number : 121-54-0
Identified uses : Laboratory chemicals, manufacture of chemical compounds
Company : Ionz

>> R&D Use only

2. Hazards Identification

GHS Classification:

Flammable liquid (category 2)
Acute toxicity, oral (Category 3)
Acute toxicity, dermal (Category 3)
Acute toxicity, inhalation (Category 3)
Specific target organ toxicity, single exposure (Category 1)

Note

>> Pictograms displayed are for 98.7% (371 of 376) of reports that indicate hazard statements. This chemical does not meet GHS hazard criteria for 1.3% (5 of 376) of reports.

Pictogram(s)

GHS Hazard Statements

>> H301 (80.1%): Toxic if swallowed [Danger Acute toxicity, oral]

>> H302 (18.4%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H314 (94.9%): Causes severe skin burns and eye damage [Danger Skin corrosion/irritation]

>> H318 (45.2%): Causes serious eye damage [Danger Serious eye damage/eye irritation]

>> H400 (94.1%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]

>> H410 (83.2%): Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P260, P264, P264+P265, P270, P273, P280, P301+P316, P301+P317, P301+P330+P331, P302+P361+P354, P304+P340, P305+P354+P338, P316, P317, P321, P330, P363, P391, P405, and P501

Health Hazards:

>> SYMPTOMS: Symptoms of exposure to this compound may include vomiting, collapse, convulsions and coma. Other symptoms may include corrosion or injury to the mucous membranes. It may cause nausea, esophageal damage and necrosis, hypotension and death. It may also cause dyspnea, cyanosis, paralysis of respiratory muscles possibly leading to asphyxia, and central nervous system depression (possibly with convulsions or preceded by excitement). It has depolarizing muscle relaxant properties. It can cause irritation to the skin, eyes, mucous membranes and upper respiratory tract. Intravenous or intrauterine administration may cause hemolysis.

>> ACUTE/CHRONIC HAZARDS: This compound is highly toxic by ingestion. It is also harmful by inhalation or skin absorption. It is an irritant of the skin, eyes, mucous membranes, and upper respiratory tract. When heated to

decomposition this chemical emits very toxic fumes of carbon monoxide, carbon dioxide, nitrogen oxides and hydrogen chloride gas. (NTP, 1992)

>> Flash point data for this chemical are not available. It is probably combustible. (NTP, 1992)

>> Combustible. Gives off irritating or toxic fumes (or gases) in a fire.

3. Composition/Information On Ingredients

Chemical name : Benzethonium Chloride
CAS Number : 121-54-0
Molecular Formula : C27H42ClNO2
Molecular Weight : 448.1000 g/mol

4. First Aid Measures

First Aid:

>> EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.

>> SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. IMMEDIATELY call a hospital or poison control center even if no symptoms (such as redness or irritation) develop. IMMEDIATELY transport the victim to a hospital for treatment after washing the affected areas.

>> INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing.

>> INGESTION: DO NOT INDUCE VOMITING. Corrosive chemicals will destroy the membranes of the mouth, throat, and esophagus and, in addition, have a high risk of being aspirated into the victim's lungs during vomiting which increases the medical problems. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. IMMEDIATELY transport the victim to a hospital. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. Transport the victim IMMEDIATELY to a hospital. (NTP, 1992)

First Aid Measures

Inhalation First Aid

>> Fresh air, rest.

Skin First Aid

>> Remove contaminated clothes. Rinse and then wash skin with water and soap.

Eye First Aid

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

Ingestion First Aid

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

5. Fire Fighting Measures

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

>> Use water spray, powder.

6. Accidental Release Measures

Spillage Disposal:

Methods for containment and safety measures to protect workers dealing with a spillage of this chemical.

>> 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

Safe Storage:

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

Storage Conditions:

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

8. Exposure Control/ Personal Protection

Effects of Short Term Exposure:

>> The substance is corrosive to the eyes. The substance is irritating to the skin.

Effects of Long Term Exposure:

>> Repeated or prolonged contact with skin may cause dermatitis.

Fire Prevention

>> NO open flames.

Inhalation Prevention

>> Use ventilation (not if powder).

Skin Prevention

>> Protective gloves.

Eye Prevention

>> Wear safety goggles.

Ingestion Prevention

>> Do not eat, drink, or smoke during work.

9. Physical And Chemical Properties

Molecular Weight:

>> 448.1

Exact Mass:

>> 447.2904073

Physical Description:

>> 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)

>> COLOURLESS OR WHITE HYGROSCOPIC SOLID IN VARIOUS FORMS.

Color/Form:

>> COLORLESS CRYSTALS

Odor:

>> MILD ODOR

Taste:

The sensation of flavor perceived in the mouth and throat on contact with a substance.

>> VERY BITTER TASTE

Melting Point:

>> 327 to 331 °F (NTP, 1992)

>> 160-165 °C

Solubility:

>> 10 to 50 mg/mL at 64 °F (NTP, 1992)

>> Solubility in water: very good

LogP:

>> 4.0

Decomposition:

>> When heated to decomposition it emits very toxic fumes of /hydrogen choride and nitrogen oxides/.

pH:

pH is an expression of hydrogen ion concentration in water. Specifically, pH is the negative logarithm of hydrogen ion (H+) concentration (mol/L) in an aqueous solution. The term is used to indicate basicity or acidity of a solution on a scale of 0 to 14, with pH 7 being neutral.

>> PH OF 1% AQ SOLN IS BETWEEN 4.8 & 5.5

Refractive Index:

>> INDEX OF REFRACTION: 1.5101 @ 25 °C/D; INDEX OF REFRACTION FALLS ON REPETITION

Collision Cross Section:

Collision cross section (CCS) represents the effective area for the interaction between an individual ion and the neutral gas through which it is traveling (e.g., in ion mobility spectrometry (IMS) experiments). It quantifies the probability of a collision taking place between two or more particles.

>> 210.3 Å² [M+H]+ [CCS Type: TW; Method: calibrated with polyalanine and drug standards]

10. Stability And Reactivity

>> Hygroscopic. May be sensitive to prolonged exposure to air. Water soluble.

11. Toxicological Information

Exposure Routes:

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

Skin Exposure

>> Redness. Pain.

Eye Exposure

>> Redness. Blurred vision. Pain. Severe burns.

Ingestion Exposure

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

Adverse Effects:

An adverse effect is an undesired harmful effect resulting from a medical treatment or other intervention.

>> Neurotoxin - Other CNS neurotoxin

>> Occupational hepatotoxin - Secondary hepatotoxins: the potential for toxic effect in the occupational setting is based on cases of poisoning by human ingestion or animal experimentation.

>> Methemoglobinemia - The presence of increased methemoglobin in the blood; the compound is classified as secondary toxic effect

>> Dermatotoxin - Skin burns.

>> Skin Sensitizer - An agent that can induce an allergic reaction in the skin.

Human Toxicity Excerpts:

>> ... USED AS SPERMATOCIDES ... CAN CAUSE VAGINAL IRRITATION, WITH BURNING SENSATIONS & ITCHING.

Non-Human Toxicity Excerpts:

>> ... CONCN OF 0.1% TO 1.0% IN WATER HAVE BEEN SIGNIFICANTLY IRRITATING OR INJURIOUS TO RABBIT EYE ... .

National Toxicology Program Studies:

Reports from the National Toxicology Program, an interagency program supported by three government agencies (NIH, FDA, and CDC) within the Department of Health and Human Services. This program plays a critical role in generating, interpreting, and sharing toxicological information about chemicals of public health concerns.

>> ... Male and female F344/N rats and B6C3FI mice were topically administered benzethonium chloride (greater than 98% pure) for ... 2 yr. ... 2 YEAR STUDY IN RATS: Groups of 60 male and 60 female F344/N rats were topically administered 0, 0.15, 0.5, or 1.5 mg benzethonium chloride/kg body weight 5 days/wk for 103 wk. ... 2 YEAR STUDY IN MICE: Groups of 60 male and 60 female B6C3F1 mice were topically administered 0, 0.15, 0.5, or 1.5 mg benzethonium chloride/kg body weight 5 days/wk for 103 wk. Doses were administered in ethanol, and dose volumes were adjusted weekly according to the average body weights of the groups. ... CONCLUSIONS: Under the conditions of these 2 yr 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 activit,v in male or female B6C3F1 mice receiving 0.15, 0.5, or 1.5 mg/kg.

12. Ecological Information

ICSC Environmental Data:

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

13. Disposal Considerations

Spillage Disposal

>> 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.

14. Transport Information

DOT

Benzethonium Chloride

IATA

Benzethonium Chloride

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15. Regulatory Information

Regulatory Information

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 - Toxicity Undefined

>> Authoritative List - CECBP - Priority Chemicals

>> Report - if used as a fragrance or flavor ingredient

REACH Registered Substance

>> Status: Active Update: 28-04-2022 https://echa.europa.eu/registration-dossier/-/registered-dossier/20277

>> Status: Active Update: 09-12-2020 https://echa.europa.eu/registration-dossier/-/registered-dossier/16540

New Zealand EPA Inventory of Chemical Status

>> Benzethonium chloride: Does not have an individual approval but may be used under an appropriate group standard

16. Other Information

Other Safety Information

Chemical Assessment

>> IMAP assessments - Benzenemethanaminium, N,N-dimethyl-N-[2-[2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethoxy]ethyl]-, chloride: Human health tier II assessment

"The information provided is believed to be accurate but is not comprehensive and should be used as a reference. It reflects our current knowledge and is intended for safety guidance related to the product. This document does not constitute a warranty of the product's properties. Ionz is not responsible for any damages resulting from handling or contact with the product incorrectly."