SAFETY DATA SHEET

Updated on 08/12/2024

1. Material Identification

Product Name : Tris(2,3-dibromopropyl) phosphate
Catalog Number : io-3179
CAS Number : 126-72-7
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)

Pictogram(s)

GHS Hazard Statements

>> H302 (100%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H315 (92.7%): Causes skin irritation [Warning Skin corrosion/irritation]

>> H350 (92.7%): May cause cancer [Danger Carcinogenicity]

>> H400 (92.7%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]

Precautionary Statement Codes

>> P203, P264, P270, P273, P280, P301+P317, P302+P352, P318, P321, P330, P332+P317, P362+P364, P391, P405, and P501

Health Hazards:

>> SYMPTOMS: Symptoms of exposure to this compound include gastrointestinal irritation, nausea, vomiting, headache, dizziness, central nervous system depression testicular atrophy, chronic lung disease, kidney damage and liver damage. It can cause eye irritation and severe skin irritation. It can also cause skin sensitization.

>> ACUTE/CHRONIC HAZARDS: This compound can be absorbed by human skin. It is an eye and severe skin irritant. It may be a CHOLINESTERASE INHIBITOR. When heated to decomposition it emits very toxic fumes of bromine and phosphorus oxides. (NTP, 1992)

>> This chemical is combustible. (NTP, 1992)

>> Combustible under specific conditions.

3. Composition/Information On Ingredients

Chemical name : Tris(2,3-dibromopropyl) phosphate
CAS Number : 126-72-7
Molecular Formula : C9H15Br6O4P
Molecular Weight : 697.6000 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. IMMEDIATELY call a physician and be prepared to transport the victim to a hospital even if no symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop. 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. If the victim is conscious and not convulsing, administer a slurry of activated charcoal in water and simultaneously 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. IMMEDIATELY transport the victim to a hospital.

>> OTHER: Since this chemical is a known or suspected carcinogen you should contact a physician for advice regarding the possible long term health effects and potential recommendation for medical monitoring. Recommendations from the physician will depend upon the specific compound, its chemical, physical and toxicity properties, the exposure level, length of exposure, and the route of exposure. (NTP, 1992)

First Aid Measures

Skin First Aid

>> 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. 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 in large amounts, foam, alcohol-resistant foam, carbon dioxide.

6. Accidental Release Measures

Isolation and Evacuation:

Isolation and evacuation measures to take when a large amount of this chemical is accidentally released in an emergency.

>> Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]:

>> IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

>> SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.

>> FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

Spillage Disposal:

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

>> Personal protection: chemical protection suit and filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

7. Handling And Storage

Safe Storage:

>> Separated from food and feedstuffs.

Storage Conditions:

>> PRECAUTIONS FOR "CARCINOGENS": Storage site should be as close as practicable to lab in which carcinogens are to be used, so that only small quantities required for ... expt need to be carried. Carcinogens should be kept in only one section of cupboard, explosion-proof refrigerator, or freezer (depending on chemicophysical properties ...) that bears appropriate label. An inventory ... should be kept, showing quantity of carcinogen & date it was acquired ... . Facilities for dispensing ... should be contiguous to storage area. /Chemical Carcinogens/

8. Exposure Control/ Personal Protection

Inhalation Risk:

>> Evaporation at 20 °C is negligible; a harmful concentration of airborne particles can, however, be reached quickly when dispersed.

Effects of Long Term Exposure:

>> This substance is probably carcinogenic to humans.

Fire Prevention

>> NO open flames.

Exposure Prevention

>> AVOID ALL CONTACT!

Skin Prevention

>> Protective clothing. Protective gloves.

Eye Prevention

>> Wear face shield or eye protection in combination with breathing protection.

Ingestion Prevention

>> Do not eat, drink, or smoke during work. Wash hands before eating.

9. Physical And Chemical Properties

Molecular Weight:

>> 697.6

Exact Mass:

>> 697.57467

Physical Description:

>> Tris(2,3-dibromopropyl) phosphate is a clear colorless to pale yellow viscous liquid. (NTP, 1992)

>> COLOURLESS VISCOUS LIQUID.

Color/Form:

>> Viscous, pale yellow liquid

Melting Point:

>> FP: 5.5 °C

>> 5.5 °C

Flash Point:

>> greater than 234 °F (NTP, 1992)

>> >110 °C

Solubility:

>> less than 1 mg/mL at 68 °F (NTP, 1992)

>> Solubility in water, g/100ml at 20 °C: 0.063

Density:

>> 2.27 at 77 °F (NTP, 1992) - Denser than water; will sink

>> Relative density (water = 1): 2.27

Vapor Pressure:

>> 0.00019 mmHg at 77 °F (NTP, 1992)

>> Vapor pressure, Pa at 25 °C: 0.019

LogP:

>> log Kow = 4.29

>> 4.29

Stability/Shelf Life:

>> Major decomp begins at 308 °C; stable in sunlight.

Decomposition:

>> When heated to decomposition it emits very toxic fumes of /bromides/ and /phosphorus oxides/.

>> 200 °C. This produces toxic and corrosive fumes including hydrogen bromide and phosphorus oxides. Reacts with acids and bases.

Viscosity:

>> High purity grade: 3900-4200 centistokes at 25 °C; low purity grade: 1400-1700 centistokes at 25 °C

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.

>> High-purity & low-purity grades: acid number (mg KOH/g)= 0.05 maximum

Refractive Index:

>> Index of refraction: 1.5772 @ 20 °C/D

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.

>> 197.25 Å² [M+H]+

>> 206.37 Å² [M+Na]+

>> 206.9 Å² [M+Na]+

10. Stability And Reactivity

>> Insoluble in water.

11. Toxicological Information

RAIS Toxicity Values:

This section provides the Chemical toxicity information from the Risk Assessment Information System.

Inhalation Unit Risk (IUR) (ug/m^3)^-1

>> 0.00066

Inhalation Unit Risk Reference

>> CALEPA

Oral Slope Factor (CSFo)(mg/kg-day)^-1

>> 2.2999999999999998

Oral Slope Factor Reference

>> CALEPA

Evidence for Carcinogenicity:

Evidence that this chemical does or may cause cancer. The information here is collected from various sources by the Hazardous Substances Data Bank (HSDB).

>> Evaluation: There is inadequate evidence in humans for the carcinogenicity of tris(2,3-dibromopropyl)phosphate. There is sufficient evidence in experimental animals for the carcinogenicity of tris(2,3-dibromopropyl)phosphate. Overall evaluation: Tris(2,3-dibromopropyl)phosphate is probably carcinogenic to humans (Group 2A). In making the overall evaluation, the Working Group took into consideration that tris(2,3-dibromopropyl)phosphate is consistently active in a wide range of mammalian in vivo and in vitro test systems.

Carcinogen Classification:

This section provides the International Agency for Research on Cancer (IARC) Carcinogenic Classification and related monograph links. In the IARC Carcinogenic classification, chemicals are categorized into four groups: Group 1 (carcinogenic to humans), Group 2A (probably carcinogenic to humans), Group 2B (possibly carcinogenic to humans), and Group 3 (not classifiable as to its carcinogenicity to humans).

IARC Carcinogenic Agent

>> Tris(2,3-dibromopropyl) phosphate

IARC Carcinogenic Classes

>> Group 2A: Probably carcinogenic to humans

IARC Monographs

>> Volume 20: (1979) Some Halogenated Hydrocarbons

>> Volume Sup 7: Overall Evaluations of Carcinogenicity: An Updating of IARC Monographs Volumes 1 to 42, 1987; 440 pages; ISBN 92-832-1411-0 (out of print)

>> Volume 71: (1999) Re-evaluation of Some Organic Chemicals, Hydrazine and Hydrogen Peroxide (Part 1, Part 2, Part 3)

Additional information

>> NB Overall evaluation upgraded to Group 2A with supporting evidence from other relevant data

Exposure Routes:

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

Ingestion Exposure

>> See Effects of long-term or repeated exposure.

Adverse Effects:

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

>> 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.

>> IARC Carcinogen - Class 2: International Agency for Research on Cancer classifies chemicals as probable (2a), or possible (2b) human carcinogens.

>> NTP Carcinogen - Reasonably anticipated to be a human carcinogen.

Antidote and Emergency Treatment:

>> /SRP:/ Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Phosphorus and related compounds/

Human Toxicity Excerpts:

>> /HUMAN EXPOSURE STUDIES/ In ... study with undiluted tris(2,3-dibromopropyl)phosphate, /skin/ sensitization reactions occurred in 8/24 subjects; with a concn of 20% in petroleum jelly, 2/25 subjects were sensitized.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ In rabbits, admin of 0.22 g/animal to the eye or 1.1 g/animal to the skin caused no irritation. No evidence of skin sensitization was seen in guinea pigs.

Non-Human Toxicity Values:

>> LD50 Rat oral 5.24 g/kg body wt /tris(2,3-dibromo-1-propyl) phosphate less than 1% volatile impurities/.

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.

>> A bioassay of technical grade tris-(2,3-dibromopropyl)phosphate (TBP) for possible carcinogenicity was conducted using Fischer 344 rats and B6C3F1 mice. TBP was administered in the feed, at either of two concentrations, to groups of 55 male and 55 female rats, and 50 male and 50 female mice. The high and low dietary concentrations of TBP administered were, respectively, 100 and 50 ppm for the male and female rats, and 1,000 and 500 ppm for the male and female mice. After a 103 wk dosing period, observation of the rats and mice continued for 1 or 2 additional wk. For each species, 55 animals of each sex were placed on test as controls. ... Under the conditions of this study, orally administered TBP was carcinogenic for B6C3F1 mice, causing incr incidences of tumors in livers, lungs, stomachs of female mice and in kidneys, lungs, and stomachs of male mice. TBP was also carcinogenic in Fischer 344 rats, causing incr incidence of kidney tumors in both sexes. Levels of Evidence of Carcinogenicity: Male Rats: Positive; Female Rats: Positive; Male Mice: Positive; Female Mice: Positive.

12. Ecological Information

Resident Soil (mg/kg)

>> 2.80e-01

Industrial Soil (mg/kg)

>> 1.30e+00

Resident Air (ug/m3)

>> 4.30e-03

Industrial Air (ug/m3)

>> 1.90e-02

Tapwater (ug/L)

>> 6.80e-03

MCL (ug/L)

>> 5.00e+01

Risk-based SSL (mg/kg)

>> 1.30e-04

Oral Slope Factor (mg/kg-day)-1

>> 2.30e+00

Inhalation Unit Risk (ug/m3)-1

>> 6.60e-04

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Soil Saturation Concentration (mg/kg)

>> 4.67e+02

ICSC Environmental Data:

>> The substance is toxic to aquatic organisms.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SOIL: Tris(2,3-dibromo-1-propyl) phosphate was identified, not quantified, in Arkansas soil(1).

13. Disposal Considerations

Spillage Disposal

>> Personal protection: chemical protection suit and filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Disposal Methods

>> Generators of waste (equal to or greater than 100 kg/month) containing this contaminant, EPA hazardous waste number U235, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

>> PRECAUTIONS FOR "CARCINOGENS": There is no universal method of disposal that has been proved satisfactory for all carcinogenic compounds, & specific methods of chem destruction ... published have not been tested on all kinds of carcinogen-containing waste. ... Summary of avail methods & recommendations ... /given/ must be treated as guide only. /Chemical Carcinogens/

>> PRECAUTIONS FOR "CARCINOGENS": ... Incineration may be only feasible method for disposal of contaminated laboratory waste from biological expt. However, not all incinerators are suitable for this purpose. The most efficient type ... is probably the gas-fired type, in which a first stage combustion with a less than stoichiometric air:fuel ratio is followed by a second stage with excess air. Some ... are designed to accept ... aqueous & organic solvent solutions, otherwise it is necessary ... to absorb soln onto suitable combustible material, such as sawdust. Alternatively, chem destruction may be used, esp when small quantities ... are to be destroyed in laboratory. /Chemical Carcinogens/

>> PRECAUTIONS FOR "CARCINOGENS": HEPA (high-efficiency particulate arrestor) filters ... can be disposed of by incineration. For spent charcoal filters, the adsorbed material can be stripped off at high temp & carcinogenic wastes generated by this treatment conducted to & burned in an incinerator. ... LIQUID WASTE: ... Disposal should be carried out by incineration at temp that ... ensure complete combustion. SOLID WASTE: Carcasses of lab animals, cage litter, & misc

solid wastes ... should be disposed of by incineration at temp high enough to ensure destruction of chem carcinogens or their metabolites. /Chemical Carcinogens/

>> For more Disposal Methods (Complete) data for TRIS(2,3-DIBROMO-1-PROPYL) PHOSPHATE (7 total), please visit the HSDB record page.

14. Transport Information

DOT

Tris(2,3-dibromopropyl) phosphate

Reportable Quantity of 10 lb or 4

IATA

Tris(2,3-dibromopropyl) phosphate

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15. Regulatory Information

Regulatory Information

The Australian Inventory of Industrial Chemicals

>> Chemical: 1-Propanol, 2,3-dibromo-, phosphate (3:1)

>> Conditions Of Use:

>> This chemical must only be introduced for research and development purposes.

>> Specific Information Requirement: Obligations to provide information apply. You must tell us within 28 days if the circumstances of your importation or manufacture (introduction) are different to those in our assessment.

California Safe Cosmetics Program (CSCP) Reportable Ingredient

>> Hazard Traits - Carcinogenicity; Hazard Trait Under Review

>> Authoritative List - CECBP - Priority Chemicals; IARC Carcinogens - 2A; NTP RoC - reasonable; Prop 65

>> Report - regardless of intended function of ingredient in the product

REACH Restricted Substance

>> Restricted substance: Tris (2,3 dibromopropyl) phosphate

>> EC: 204-799-9

16. Other Information

Toxic Combustion Products:

Toxic products (e.g., gases and vapors) produced from the combustion of this chemical.

>> When heated to decomposition it emits very toxic fumes of Br- /bromides/ and POx /phosphorus oxides/.

Other Safety Information

Chemical Assessment

>> PEC / SN / Other assessments - Polybrominated flame retardants (PBFRs): Health and Environment

>> PEC / SN / Other assessments - Tris(2,3-dibromopropyl) phosphate (TBPP): Health and Environment

"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. Lonz is not responsible for any damages resulting from handling or contact with the product incorrectly."