SAFETY DATA SHEET

Updated on 20/07/2024

1. Material Identification

Product Name : Quintozene
Catalog Number : io-2960
CAS Number : 82-68-8
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)

>> Warning

GHS Hazard Statements

>> H317 (100%): May cause an allergic skin reaction [Warning Sensitization, Skin]

>> H400 (100%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]

>> H410 (100%): Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P261, P272, P273, P280, P302+P352, P321, P333+P317, P362+P364, P391, and P501

Health Hazards:

>> SYMPTOMS: Symptoms of exposure to this compound may include irritation of the skin and eyes. Skin contact may result in erythema, itching, edema and formation of small vesicles. Skin sensitization may also occur. Eye contact may result in conjunctivitis and corneal injury. Kidney and liver damage may occur. Vomiting may also occur. Exposure to this type of compound can cause central nervous system stimulation, vomiting, diarrhea, paresthesia, excitement, giddiness, fatigue, tremors, convulsions, coma, pulmonary edema, hypothermia and liver, kidney and myocardial toxicity. Respiration may be initially accelerated and then later depressed. Chronic exposure to this type of compound leads to headache, loss of appetite, muscular weakness, fine tremors and apprehensive mental state.

>> ACUTE/CHRONIC HAZARDS: This compound is harmful if swallowed, inhaled or absorbed through the skin. It may cause irritation. When heated to decomposition it emits toxic fumes of chlorine, carbon monoxide, carbon dioxide, nitrogen oxides, hydrogen chloride gas and phosgene. (NTP, 1992)

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

>> Liquid formulations containing organic solvents may be flammable. Gives off irritating or toxic fumes (or gases) in a fire.

3. Composition/Information On Ingredients

Chemical name : Quintozene
CAS Number : 82-68-8
Molecular Formula : C6Cl5NO2
Molecular Weight : 295.3000 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. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment.

>> 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, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. 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

Inhalation First Aid

>> Fresh air, rest.

Skin First Aid

>> Remove contaminated clothes. Rinse skin with plenty of water or shower.

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. A water spray may also be used. (NTP, 1992)

>> In case of fire in the surroundings, use appropriate extinguishing media.

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: 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:

>> Provision to contain effluent from fire extinguishing.

Storage Conditions:

>> Store in a refrigerator or cool, dry place away from strong bases. A regulated, marked area should be established where this chemical is handled, used, or stored in compliance with OSHA standard 1910.1045.

8. Exposure Control/ Personal Protection

>> 0.5 [mg/m3]

>> 0.5 mg/m

TLV-TWA (Time Weighted Average)

>> 0.5 mg/m³ [1988]

Inhalation Risk:

>> A harmful concentration of airborne particles can be reached quickly when dispersed.

Effects of Long Term Exposure:

>> The substance may have effects on the liver. This may result in impaired functions.

Exposure Prevention

>> STRICT HYGIENE! AVOID EXPOSURE OF ADOLESCENTS AND CHILDREN!

Inhalation Prevention

>> Avoid inhalation of dust.

Skin Prevention

>> Protective gloves.

Eye Prevention

>> Wear safety spectacles.

Ingestion Prevention

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

9. Physical And Chemical Properties

Molecular Weight:

>> 295.3

Exact Mass:

>> 294.834217

Physical Description:

>> Quintozene appears as crystalline pale yellow to white solid or powder with a musty moth ball odor. Insoluble in water and denser than water. Hence sinks in water.

>> PURE: COLOURLESS CRYSTALS WITH CHARACTERISTIC ODOUR. TECHNICAL: PALE YELLOW CRYSTALS WITH CHARACTERISTIC ODOUR.

Color/Form:

>> Pale yellow crystals

Odor:

>> Musty odor

Boiling Point:

>> 622 °F at 760 mmHg (with some decomposition) (NTP, 1992)

>> 328 °C

Melting Point:

>> 295 °F (NTP, 1992)

>> 146 °C

Solubility:

>> less than 1 mg/mL at 72 °F (NTP, 1992)

>> Solubility in water, g/100ml at 20 °C: 0.00004

Density:

>> 1.718 at 77 °F (NTP, 1992) - Denser than water; will sink

>> 1.7 g/cm³

Vapor Density:

>> 10.2 (NTP, 1992) - Heavier than air; will sink (Relative to Air)

>> Relative vapor density (air = 1): 10.2

Vapor Pressure:

>> 0.013 mmHg at 77 °F (NTP, 1992)

>> Vapor pressure, Pa at 20 °C: 0.007

LogP:

>> log Kow = 4.22

>> 4.77

Stability/Shelf Life:

>> STABLE IN SUNLIGHT

Corrosivity:

The ability of a chemical to damage or destroy other substances when it comes into contact.

>> NON-CORROSIVE

10. Stability And Reactivity

>> Insoluble in water.

11. Toxicological Information

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).

>> Cancer Classification: Group C Possible Human Carcinogen

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

>> Quintozene (Pentachloronitrobenzene)

IARC Carcinogenic Classes

>> Group 3: Not classifiable as to its carcinogenicity to humans

IARC Monographs

>> Volume 5: (1974) Some Organochlorine Pesticides

>> 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)

>> 3, not classifiable as to its carcinogenicity to humans. (L135)

Exposure Routes:

>> The substance can be absorbed into the body by inhalation of its aerosol.

Target Organs:

Organs that are affected by exposure to this chemical. Information in this section reflects human data unless otherwise noted.

>> Hepatic

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.

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

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

>> ACGIH Carcinogen - Not Classifiable.

Toxicity Data:

>> LC50 (rat) = 1,400 mg/m3

Interactions:

>> Pentachloronitrobenzene (PCNB) and $HgCl_2$, PCNB and $CdCl_2$, and hexachlorobenzene (HCB) and $HgCl_2$ were investigated for their acute oral toxicity in rats, individually and as combinations in various ratios of the organochlorine pesticides to the heavy metal chlorides. The toxicity of mixtures of low dosages of the pairs tested was higher than the sum of the toxicities produced by the individual doses. At increased dosages of the components in the combinations PCNB-$HgCl_2$ and PCNB-$CdCl_2$, the combined lethality tended towards the sums of the effects of the individual doses.

Antidote and Emergency Treatment:

>> Gastrointestinal decontamination. If a large amount of the fungicide has been ingested in the last few hours, and if copious vomiting has not already occurred, it may be reasonable to consider GI decontamination. Activated charcoal can be used along with the addition of the cathartic sorbitol to the charcoal slurry. If sorbitol is given separately, it should be diluted with an equal volume of water before administration. No more than one dose of sorbitol is recommended and it should be used with caution in children and the elderly. If contact with the toxicant has been minimal (for example, oral contamination only, promptly flushed out of the mouth), administration of charcoal without a cathartic, followed by careful observation of the patient, probably represents optimal management. /Substituted benzenes/

Human Toxicity Excerpts:

>> /HUMAN EXPOSURE STUDIES/ Skin sensitivity tests in man revealed no irritation after 48 hr contact, but sensitivity reaction occurred in 20% of subjects after second skin exposure.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ Large doses induce vomiting in dogs.

Non-Human Toxicity Values:

>> LD50 Rat oral greater than 12000 mg/kg

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 pentachloronitrobenzene for possible carcinogenicity was conducted using Osborne-Mendel rats and B6C3F1 mice. /The cmpd/ was administered in the feed, at either of two concentrations, to groups of 50 male and 50 female animals of each species. The time weighted avg dietary concn of PCNB were, respectively, 10,064 and 5,417 ppm for male rats, 14,635 and 7,875 ppm for female rats, 5,213 and 2,606 for male mice, and 8,187 and 4,093 ppm for female mice. After a 78 wk period of cmpd administration, observation of the rats continued for an additional 33-35 wk and observation of the mice continued for 14-15 additional wk. For each species, 20 animals of each sex were placed on test as controls and fed only the basal diet. No rare or unusual tumors were observed during the histopathologic examinations and no statistically significant positive associations were demonstrated between chemical administration and the incidence of neoplasms in either sex of either species. Under the conditions of this bioassay, pentachloronitrobenzene was not carcinogenic in either Osborne-Mendel rats or B6C3F1 mice. Levels of Evidence of Carcinogenicity: Male Rats: Negative; Female Rats: Negative; Male Mice: Negative; Female Mice: Negative.

TSCA Test Submissions:

Under the Toxic Substances Control Act (TSCA), EPA has broad authority to issue regulations designed to require manufacturers (including importers) or processors to test chemical substances and mixtures for health and environmental effects. This section provides information on test reports submitted for this chemical under TSCA.

>> Pentachloronitrobenzene (CAS# 82-68-8) was evaluated for eye irritation. The test substance was instilled into the conjunctival sac of two pairs of rabbit eyes at a dose level of 10 mg of powder or 0.1 ml of a 10% suspension in propylene glycol, respectively. Twenty seconds after treatment one eye of each pair was washed for one minute. The other eye was not washed. Ocular effects in the unwashed eye at 10 mg included mild conjunctivae inflammation. Ocular effects of washed and unwashed eyes at 0.1 ml included injections of blood vessels on the iris and mild conjunctivae inflammation on day of treatment. The unwashed eye also had a fibrous discharge of the conjunctivae on day 1. The test substance caused no corneal injury and only mild transient irritation of the conjunctivae and iris.

12. Ecological Information

Resident Soil (mg/kg)

>> 2.70e+00

Industrial Soil (mg/kg)

>> 1.30e+01

Tapwater (ug/L)

>> 1.20e-01

MCL (ug/L)

>> 2.00e+02

Risk-based SSL (mg/kg)

>> 1.50e-03

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

>> 2.60e-01

Chronic Oral Reference Dose (mg/kg-day)

>> 3.00e-03

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

ICSC Environmental Data:

>> The substance is very toxic to aquatic organisms. Bioaccumulation of this chemical may occur in fish. This substance does enter the environment under normal use. Great care, however, should be taken to avoid any additional release, for example through inappropriate disposal.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SOIL: Pentachloronitrobenzene concentrations (ppm dry weight) in cropland soils were: 2.61 (Oklahoma), 0.22 (Tennessee), and 0.98 (North Carolina)(1). Pentachloronitrobenzene concentrations of up to 27.0 mg/kg and 12.2 mg/kg were found in the soil of forest tree nurseries and in agricultural soil, respectively, in Finland(2). In Denmark, pentachloronitrobenzene concn in field samples of soil ranged from 0.01 to 25.25 mg/kg (3). Pentachloronitrobenzene concentrations in greenhouse soils in W Germany ranged from 0.019 to 1.020 ppm(4). Maximum pentachloronitrobenzene concentrations found in W German soils were 55.6 ppm (chicory cultivation) and 8.4 ppm (lettuce cultivation)(5). Pentachloronitrobenzene concentrations in soil were similar to those of river sediment at an intensively farmed area in Tsumagoi, Japan; pentachloronitrobenzene was concentrated 5000-10,000 times over levels in river water(6). Soil samples randomly collected from five locations at Humrat Al-Sahn, Jordan in 1998(1). Pentachloronitrobenzene concentrations were reported as 0.02 ppm in two of the five sites (WDA site: pH 7.9, 50.0% sand, 17.5% silt, 32.5% clay; WDW site: pH 7.8, 50.0% sand, 12.5% silt, 37.5% clay)(7). It was not detected at sites with the following characteristics: GHR site: pH 7.9, 65% sand, 17.5% silt, 17.5% clay; WUR site: pH 8.1, 37.5% sand, 30.0% silt, 32.5% clay; WDB site: pH 7.9, 50.0% sand, 17.5% silt, 32.5% clay)(7).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

>> Pentachloronitrobenzene was detected in 1 US fish and shellfish sample during the fiscal years of 1970-76(1). Bottom feeding and game fish samples collected from one of 400 sites in the US between 1986 and 1989 contained pentachloronitrobenzene at a maximum concentration of 10 ng/g and a mean concentration of 0.09 ng/g(2).

Average Daily Intake:

The average amount of the compound taken into the body through eating, drinking, or breathing.

>> The average daily intake of pentachloronitrobenzene in the US during the fiscal years 1971-76 was 9X10-7 mg/kg body wt/ day(1). Average daily intakes (ug/kg body wt/day) of pentachloronitrobenzene in US total diet studies for fiscal years 1977 and 1978 were: 0.0010 and 0.0007 for adults(2), 0.0014 and 0.0045 for infants(3), and 0.0029 and 0.0026 for toddlers(3). Average daily intakes (ug/kg body wt/day) of pentachloronitrobenzene in US total diet studies for fiscal years 1976 and 1979 were: 0.002 and 0.002 for infants and 0.004 and 0.002 for toddlers, respectively(4). Average daily intakes (ug/kg body wt/day) of pentachloronitrobenzene in US total diet studies for fiscal years 1980 and 1981/82 were: 0.001 and 0.001 for adults(5), not detected and 0.003 for infants, and 0.001 and 0.001 for toddlers, respectively(6). The average daily intake of pentachloronitrobenzene in Belgium from 1991 to 1993 from 3698 samples of food was determined to be 0.007 mg/kg/day(7).

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.

Disposal Methods

>> [40 CFR 240-280, 300-306, 702-799 (7/1/2006)] Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number U185, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

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>> Drift and runoff may be hazardous to aquatic organisms in water adjacent to treated areas. Do not contaminate water when disposing of equipment wash waters or rinsate.

>> It has been observed that the product decomposes readily when burned with polyethylene. The cmpd is very stable in soil as would be expected on the basis of the polychlorinated aromatic structure. Recommendable method: Incineration. Not recommendable methods: Open burning, use as boiler fuel. Peer-review: Ensure adequate fuel supply. (Peer-review conclusions of an IRPTC expert consultation (May 1985))

>> For more Disposal Methods (Complete) data for PENTACHLORONITROBENZENE (7 total), please visit the HSDB record page.

14. Transport Information

DOT

Quintozene
9
UN Pack Group: III
Reportable Quantity of 100 lb or 45

IATA

Quintozene
9,
UN Pack Group: III

15. Regulatory Information

Regulatory Information

New Zealand EPA Inventory of Chemical Status

>> Quintozene: Does not have an individual approval but may be used as a component in a product covered by a group standard. It is not approved for use as a chemical in its own right.

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 HIGHLY TOXIC FUMES OF CHLORIDES AND OXIDES OF NITROGEN.

Other Safety Information

Chemical Assessment

>> IMAP assessments - Benzene, pentachloronitro-: Environment tier I assessment

>> IMAP assessments - Benzene, pentachloronitro-: Human health tier I 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."