ionz

SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : trans-1,4-Dichlorobutene
Catalog Number : io-2151
CAS Number : 110-57-6
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

>> H226 (47.5%): Flammable liquid and vapor [Warning Flammable liquids]

>> H301+H311 (47.5%): Toxic if swallowed or in contact with skin [Danger Acute toxicity, oral; acute toxicity, dermal]

>> H301 (100%): Toxic if swallowed [Danger Acute toxicity, oral]

>> H311 (100%): Toxic in contact with skin [Danger Acute toxicity, dermal]

>> H314 (98.8%): Causes severe skin burns and eye damage [Danger Skin corrosion/irritation]

>> H330 (100%): Fatal if inhaled [Danger Acute toxicity, inhalation]

>> H350 (98.8%): May cause cancer [Danger Carcinogenicity]

>> H400 (98.8%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]

>> H410 (98.8%): Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P203, P210, P233, P240, P241, P242, P243, P260, P262, P264, P270, P271, P273, P280, P284, P301+P316, P301+P330+P331, P302+P352, P302+P361+P354, P303+P361+P353, P304+P340, P305+P354+P338, P316, P318, P320, P321, P330, P361+P364, P363, P370+P378, P391, P403+P233, P403+P235, P405, and P501

Health Hazards:

>> Inhalation of vapor irritates nose and throat. Contact with eyes causes intense irritation and tears. Contact of liquid with skin causes severe blistering and dermatitis. Ingestion causes severe irritation of mouth and stomach. (USCG, 1999)

>> Special Hazards of Combustion Products: Decomposition vapors contain phosgene and hydrogen chloride gases; both are toxic and irritating. (USCG, 1999)

3. Composition/Information On Ingredients

Chemical name : trans-1,4-Dichlorobutene
CAS Number : 110-57-6
Molecular Formula : C4H6Cl2
Molecular Weight : 124.9900 g/mol

4. First Aid Measures

First Aid:

>> INHALATION: remove from exposure; provide low-pressure oxygen if required; keep under observation until edema is ruled out.

>> EYES: irrigate immediately for 15 min.; call physician.

>> SKIN: wash immediately and thoroughly with soap and water; treat as a chemical burn.

>> INGESTION: induce vomiting; call physician. (USCG, 1999)

5. Fire Fighting Measures

>> Flashback along vapor trail may occur. /Dichlorobutene/

>> Excerpt from ERG Guide 132 [Flammable Liquids - Corrosive]:

>> Some of these materials may react violently with water.

>> SMALL FIRE: Dry chemical, CO2, water spray or alcohol-resistant foam.

>> LARGE FIRE: Water spray, fog or alcohol-resistant foam. If it can be done safely, move undamaged containers away from the area around the fire. Dike runoff from fire control for later disposal. Do not get water inside containers.

>> FIRE INVOLVING TANKS, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks in direct contact with flames. For massive fire, use unmanned master stream devices or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2024)

>> Wear positive pressure breathing apparatus and full protective clothing. Move containers from fire area if you can do so without risk. Spray containers with cooling water until well after fire is out. Isolate for one-half mile in all directions if tank car or truck is involved in a fire. For small fires, use dry chemical, carbon dioxide, spray or foam. For large fires, use water spray, fog, or foam. (EPA, 1998)

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 132 [Flammable Liquids - Corrosive]:

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

>> 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)

7. Handling And Storage

Storage Conditions:

>> Storage temperature: Ambient with open venting and equipped with a flame arrester. /Dichlorobutene/

8. Exposure Control/ Personal Protection

>> 0.005 [ppm]

9. Physical And Chemical Properties

Molecular Weight:

>> 124.99

Exact Mass:

>> 123.9846556

Physical Description:

>> 1,4-dichloro-2-butene appears as a clear colorless liquid. Burns, though may be difficult to ignite. Corrosive to tissue. Denser than water and insoluble in water. Vapors heavier than air. Used to make other chemicals.

Color/Form:

>> COLORLESS LIQUID

Odor:

>> DISTINCT ODOR

Boiling Point:

>> 313 °F at 760 mmHg (USCG, 1999)

Melting Point:

>> -54 °F (USCG, 1999)

Flash Point:

>> 53 °C

Solubility:

>> Sol in alcohol, ether, acetone, benzene

Density:

>> 1.112 at 68 °F (USCG, 1999) - Denser than water; will sink

Vapor Density:

>> 4 (EPA, 1998) - Heavier than air; will sink (Relative to Air)

Vapor Pressure:

>> 3.0 [mmHg]

Stability/Shelf Life:

>> Reacts slowly with water to form hydrochloric acid. /Dichlorobutene/

Decomposition:

>> When heated to decomposition it emits toxic fumes of /hydrogen chloride/.

Viscosity:

>> 1.293X10-3 Pa-sec @ melting point

Corrosivity:

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

>> Corrosive

Heat of Combustion:

>> -17,500 Btu/lb = -9,720 cal/g = -407x10+7 J/kg

Heat of Vaporization:

>> 130 Btu/lb = 73 cal/g = 3.1x10+5 J/kg

Surface Tension:

>> 24 dynes/cm = 0.024 N/m at 20 °C

Refractive Index:

>> Index of refraction: 1.4871 @ 25 °C

10. Stability And Reactivity

>> Highly flammable. Reacts slowly with water to form hydrochloric acid. Insoluble in water.

>> Highly Flammable

11. Toxicological Information

EPA Provisional Peer-Reviewed Toxicity Values:

This section provides the EPA Provisional Peer-Reviewed Toxicity Values (PPRTVs) and links of related assessment documents.

Chemical Substance

>> trans-1,4-Dichloro-2-butene

PPRTV Assessment

>> PDF Document

Weight-Of-Evidence (WOE)

>> Suggestive evidence of carcinogenic potential

Last Revision

>> 2008

USGS Health-Based Screening Levels for Evaluating Water-Quality:

This section provides the USGS Health-Based Screening Levels for Evaluating Water-Quality data.

Chemical

>> trans-1,4-Dichloro-2-butene

Reference

>> Smith, C.D. and Nowell, L.H., 2024. Health-Based Screening Levels for evaluating water-quality data (3rd ed.). DOI:10.5066/F71C1TWP

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).

>> A2: Suspected human carcinogen. /1,4-Dichloro-2-butene/

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

>> trans-1,4-Dichlorobutene

IARC Carcinogenic Classes

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

IARC Monographs

>> Volume 15: (1977) Some Fumigants, the Herbicides 2,4-D and 2,4,5-T, Chlorinated Dibenzodioxins and Miscellaneous Industrial Chemicals

>> 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)

Adverse Effects:

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

>> Dermatotoxin - Skin burns.

>> Lacrimator (Lachrymator) - A substance that irritates the eyes and induces the flow of tears.

>> Toxic Pneumonitis - Inflammation of the lungs induced by inhalation of metal fumes or toxic gases and vapors.

>> ACGIH Carcinogen - Suspected Human.

Toxicity Data:

>> LC50 (rat) = 86 ppm/4hr

Antidote and Emergency Treatment:

>> Stabilization: Treatment is largely supportive. Watch for respiratory depression & arrhythmias. Obtain arterial blood gases. Administer oxygen if there is evidence of altered mental status or dyspnea. Treat hypotension with volume expansion & vasopression. Use lidocaine or beta-blockers for ventricular arrhythmias. Skin: Remove contaminated clothing. Wash affected area with soap & copious amounts or water. Eye: Irrigate the eye for 15-20 min. Obtain a consultation if symptoms persist. Oral: Most of the halogenated solvents ingested in quantities of 1-2 swallows may be partially removed by ipecac-induced emesis if admin within a few hr to a patient who has not lost the gag reflex, is not seizing, is not markedly lethargic, or is not in coma. Observe the patient in the upright position to lessen the possibility of aspiration. Activated charcoal is probably ineffective. Inhalation: Move from the contaminated area. Provide a source of oxygen & prepare for mechanical ventilation. If the patient is unconscious & the pulse is absent, initiate CPR measures. Enhancement of Elimination: Maintain good ventilation. Hemodialysis or hemoperfusion are not likely to be useful because of the high lipophilic properties of these solvents. Antidote: N-acetylcysteine may restore depleted glutathione stores, but no adequate clinical studies are available to validate this possible treatment. Supportive Care: Watch for cardiac dysrhythmias, aspiration pneumonitis, hepatotoxicity, & hypoxic encephalopathy. Monitor for arrhythmia for at least 24 hr & for hepatorenal failure for about 3 days. Obtain a chest x-ray, arterial blood gas, EKG, serum creatinine, & hepatic aminotransferase. Check electrolyte imbalance daily. Treat renal failure with dialysis & hepatic failure with fresh frozen plasma, vitamin K, a low-protein diet, neomycin, & lactulose. Watch fluid & electrolyte balance. /Halogenated hydrocarbons/

Human Toxicity Excerpts:

>> AVAILABLE DATA DO NOT ALLOW AN EVALUATION OF CARCINOGENICITY ...

Non-Human Toxicity Excerpts:

>> ... 62 PPM (0.34 MG/L) GIVEN TO RATS BY INHALATION FOR 4 HR CAUSED MORTALITY IN 2/6 ANIMALS IN 14 DAYS.

Non-Human Toxicity Values:

>> LC50 Rat inhalation 86 ppm/4 hr

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.

>> Chronic toxicity and oncogenicity were evaluated in male Crl:CD(SD)BR rats exposed to 1,4-dichloro-2-butene (DCB) via inhalation at concentrations of (number of rats): 0 (160), 0.10 (150), 0.31 (150) or 1.0 ppm (128) for 6 hrs/day, 5 days/week for 3-19 months with rats surviving 19 months of exposure held without treatment for an additional 5 months. All groups exhibited infection by Corynebacterium kutscheri which especially affected the chronic toxicity portion of the tests. After adjusting for effects due to the infection, there was a statistical increase in mortality in the high dose group. There were significant dose-related increases in treated groups relative to controls in various nasal tumors (dose group(ppm)/month first observed): benign tumors in the respiratory region of the nasal cavity (1.0/10 months, 0.31/12 months, 0.10/19 months), and malignant tumors in the olfactory region (1.0/12 months, 0.31/19 months). The increase in tumor incidence was statistically significant at all exposure concentrations for benign tumors, at 1.0 ppm

for malignant tumors and at 0.3 and 1.0 ppm for both types of tumors combined. The infection did not appear to affect tumor incidence although the infection reduced the numbers of rats at risk due to an increased mortality.

12. Ecological Information

Resident Soil (mg/kg)

>> 2.10e-03

Industrial Soil (mg/kg)

>> 9.40e-03

Resident Air (ug/m3)

>> 6.70e-04

Industrial Air (ug/m3)

>> 2.90e-03

Tapwater (ug/L)

>> 1.30e-03

MCL (ug/L)

>> 4.0E+03(G)

Risk-based SSL (mg/kg)

>> 6.6e-07

Inhalation Unit Risk (ug/m3)-1

>> 4.20e-03

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Soil Saturation Concentration (mg/kg)

>> 5.54e+02

13. Disposal Considerations

Disposal Methods

>> At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

>> /1,4-Dichloro-2-butene/ may be disposed of by the use of the following incineration methods: Rotary kiln with a temperature of 820-1600 °C and a residence time of seconds for liquids and gases, and hours for solids. Liquid injection with a temperature of 650-1600 °C with a residence time of 0.1-2 seconds. Fluidized bed with a temperature of 450-980 °C with a residence time of seconds for liquids and gases, longer for solids. /1,4-Dichloro-2-butene/

>> Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number U074, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

14. Transport Information

DOT

trans-1,4-Dichlorobutene

IATA

trans-1,4-Dichlorobutene

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15. Regulatory Information

Regulatory Information

The Australian Inventory of Industrial Chemicals

>> Chemical: 2-Butene, 1,4-dichloro-

New Zealand EPA Inventory of Chemical Status

>> 2-Butylene dichloride: HSNO Approval: HSR002956 Approved with controls

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 toxic fumes of /chloride/.

Other Safety Information

Chemical Assessment

>> IMAP assessments - 2-Butene, 1,4-dichloro-: Environment tier I assessment

>> IMAP assessments - CMR chemicals not registered under REACH: 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."