

1. Material Identification

Product Name : 1,3-Dichlorobenzene

Catalog Number : io-2142

CAS Number : 541-73-1

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

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

>> H315 (36.5%): Causes skin irritation [Warning Skin corrosion/irritation]

>> H317 (35.4%): May cause an allergic skin reaction [Warning Sensitization, Skin]

>> H336 (33.1%): May cause drowsiness or dizziness [Warning Specific target organ toxicity, single exposure; Narcotic effects]

>> H411 (99.6%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P261, P264, P270, P271, P272, P273, P280, P301+P317, P302+P352, P304+P340, P319, P321, P330, P332+P317, P333+P317, P362+P364, P391, P403+P233, P405, and P501

Health Hazards:

>> INHALATION: Causes headache, drowsiness, unsteadiness. Irritating to mucous membranes. EYES: Severe irritation. SKIN: Severe irritation. INGESTION: Irritation of gastric mucosa, nausea, vomiting, diarrhea, abdominal cramps and cyanosis. (USCG, 1999)

>> Special Hazards of Combustion Products: Irritating vapors including hydrogen chloride are produced. (USCG, 1999)

>> Combustible. Gives off irritating or toxic fumes (or gases) in a fire. Above 63 °C explosive vapour/air mixtures may be formed.

3. Composition/Information On Ingredients

Chemical name : 1,3-Dichlorobenzene

CAS Number : 541-73-1

Molecular Formula : C₆H₄Cl₂

Molecular Weight : 147.0000 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. 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. 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. (NTP, 1992)

First Aid Measures

Inhalation First Aid

- >> Fresh air, rest. Refer for medical attention.

Skin First Aid

- >> Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

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

- >> Fire Extinguishing Agents: Water, foam, carbon dioxide or dry or dry chemical. (USCG, 1999)
- >> Use water spray, powder, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

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 153 [Substances – Toxic and/or Corrosive (Combustible)]:

- >> 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: filter respirator for organic gases and particulates adapted to the airborne concentration of the substance. 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. Do NOT let this chemical enter the environment.

7. Handling And Storage

Safe Storage:

- >> Provision to contain effluent from fire extinguishing. Separated from strong oxidants, aluminium and food and feedstuffs. Well closed. Store in an area without drain or sewer access.

8. Exposure Control/ Personal Protection

MAK (Maximale Arbeitsplatz Konzentration)

- >> 12 mg/m

Inhalation Risk:

- >> No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20 °C.

Effects of Short Term Exposure:

- >> The vapour is irritating to the eyes, skin and respiratory tract.

Effects of Long Term Exposure:

- >> The substance may have effects on the kidneys and liver.

Fire Prevention

- >> NO open flames. Above 63 °C use a closed system and ventilation.

Exposure Prevention

- >> PREVENT GENERATION OF MISTS!

Inhalation Prevention

- >> Use ventilation, local exhaust or breathing protection.

Skin Prevention

- >> Protective gloves.

Eye Prevention

- >> Wear safety goggles.

Ingestion Prevention

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

Exposure Control and Personal Protection

Maximum Allowable Concentration (MAK)

>> 2.0 [ppm]

9. Physical And Chemical Properties

Molecular Weight:

>> 147.00

Exact Mass:

>> 145.9690055

Physical Description:

>> M-dichlorobenzene is a colorless liquid. Sinks in water. (USCG, 1999)

>> COLOURLESS LIQUID.

Color/Form:

>> Colorless liquid

Boiling Point:

>> 343 °F at 760 mmHg (NTP, 1992)

>> 173 °C

Melting Point:

>> -12.6 °F (NTP, 1992)

>> -24.8 °C

Flash Point:

>> 146 °F (NTP, 1992)

>> 63 °C

Solubility:

>> less than 1 mg/mL at 70 °F (NTP, 1992)

>> Solubility in water: none

Density:

>> 1.2884 at 68 °F (USCG, 1999) – Denser than water; will sink

>> Relative density (water = 1): 1.288

Vapor Density:

>> 5.08 (NTP, 1992) – Heavier than air; will sink (Relative to Air)

>> Relative vapor density (air = 1): 5.1

Vapor Pressure:

>> 1 mmHg at 53.8 °F ; 5 mmHg at 102 °F; 40 mmHg at 180 °F (NTP, 1992)

>> Vapor pressure, kPa at 25 °C: 0.286

LogP:

>> log Kow = 3.53

>> 3.53

Autoignition Temperature:

>> 1198 °F (USCG, 1999)

Decomposition:

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

Viscosity:

>> 1.044 mPa.s at 25 °C

Heat of Vaporization:

>> 296.8 J/g

Surface Tension:

>> 36.20 dynes/cm

Refractive Index:

>> Index of refraction: 1.5515 at 20 °C/D

10. Stability And Reactivity

>> This compound is sensitive to moisture. Insoluble in water.

11. Toxicological Information

Toxicity Summary:

>> The liver damage caused in rats by 1,3-dichlorobenzene is accompanied by induction of xenobiotic metabolizing enzymes of the phenobarbital type. In rats, a disturbance in thyroid homoeostasis can develop by hepatic enzyme induction: 1,3-dichlorobenzene induces glucuronosyl transferases. The conjugation of the thyroid hormones thyroxine (T4) and triiodothyronine (T3) is increased by the induction of glucuronosyl transferases. This leads to an increased release of T4 and T3 in the thyroid follicles.

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

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

Chemical

>> 1,3-Dichlorobenzene

Noncancer HBSL (Health-Based Screening Level)[µg/L]

>> 500

Benchmark Remarks

>> Based on data for 1,2-Dichlorobenzene CASRN 95501

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).

>> CLASSIFICATION: D; not classifiable as to human carcinogenicity. BASIS FOR CLASSIFICATION: Based on no human data, no animal data and limited genetic data. HUMAN CARCINOGENICITY DATA: None. ANIMAL CARCINOGENICITY DATA: None. /Classification based on former EPA guidelines/

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

>> meta-Dichlorobenzene

IARC Carcinogenic Classes

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

IARC Monographs

>> Volume 73: (1999) Some Chemicals that Cause Tumours of the Kidney or Urinary Bladder in Rodents and Some Other Substances

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

Health Effects:

- >> Acute (short-term) exposure to 1,4-dichlorobenzene, via inhalation in humans, results in irritation of the skin, throat, and eyes. Chronic (long-term) 1,4-dichlorobenzene inhalation exposure in humans results in effects on the liver, skin, and central nervous system (CNS). No information is available on the reproductive, developmental, or carcinogenic effects of 1,4-dichlorobenzene in humans. A National Toxicology Program (NTP) study reported that 1,4-dichlorobenzene caused kidney tumors in male rats and liver tumors in both sexes of mice by gavage (experimentally placing the chemical in their stomachs).

Exposure Routes:

- >> The substance can be absorbed into the body by inhalation and by ingestion.
- >> Inhalation

Inhalation Exposure

- >> Cough. Drowsiness. Nausea. Sore throat. Vomiting.

Skin Exposure

- >> Redness. Pain.

Eye Exposure

- >> Redness. Pain.

Ingestion Exposure

- >> Burning sensation. Diarrhoea. Nausea. Vomiting.

Adverse Effects:

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

- >> Neurotoxin – Acute solvent syndrome
- >> 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.

Toxicity Data:

- >> LC50 (rat) = 2,965 ppm/6h

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. /Lindane and related compounds/

Human Toxicity Excerpts:

- >> /HUMAN EXPOSURE STUDIES/ In 2 subjects with chronic lymphoid leukemia, 1 had been exposed to glue containing 2% ortho-dichlorobenzene from 1945-1961, and other had been exposed from 1940-1950 to solvent containing ortho- (80%), meta- (2%) and para- (15%) dichlorobenzene ... /SRP- actual carcinogenic agent in these exposures has not been identified/ (Girard et al, 1969).

Non-Human Toxicity Excerpts:

- >> /LABORATORY ANIMALS: Acute Exposure/ Rats were treated with each isomer of dichlorobenzene (DCB) in an oral dose of 250 mg/kg once daily for 3 days. Activities of aminopyrine demethylase and aniline hydroxylase were enhanced markedly by treatment with m-dichlorobenzene, whereas cytochrome content was not altered significantly by treatment with any isomers of dichlorobenzene. Delta-amino levulinic acid synthetase activity was enhanced 63, 32 and 42% by treatment with o-, m-, p-DCB respectively, but these enhancements were not paralleled by cytochrome p450 change.

Non-Human Toxicity Values:

- >> LD50 Rat (Sprague-Dawley male) oral (gavage) 1,200 mg/kg

Populations at Special Risk:

- >> Persons with existing pathology (hepatic, renal, central nervous system, blood), or metabolic disorders, who are taking certain drugs (hormones, or otherwise metabolically active) or who are otherwise exposed to dichlorobenzenes or to related (chemically or biologically) chemicals, by such means as occupation or domestic use or abuse ... might well be considered at increased risk from exposure to dichlorobenzenes. /Dichlorobenzenes/

12. Ecological Information

ICSC Environmental Data:

>> The substance is toxic to aquatic organisms. Bioaccumulation of this chemical may occur in fish.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SEDIMENT: 1,3-Dichlorobenzene was detected in the sediment of Lake Ketelmeer, Netherlands at concns of 280 and 110 ng/kg(1). Mean 1,3-dichlorobenzene concns of 2, 2, 4 and 74 ppb were detected in the superficial sediments from Lakes Superior, Huron, Erie, and Ontario, respectively(2). 1,3-Dichlorobenzene was detected at concns of 0–51 ng/g in sediment from Ise Bay, Japan(3). 1,3-Dichlorobenzene was identified, not quantified, in the sediment of 7 rivers and ports in Niigata, Japan(4). 1,3-Dichlorobenzene was detected at concns of 16–19 ng/g in suspended sediment from Lake Ontario, at depths of 20–68 meters and an avg concn of 15 ng/g for the bottom sediment(5). 1,3-Dichlorobenzene was identified, not quantified, in sediment from Dokai Bay, Japan(6). 1,3-Dichlorobenzene was detected at median concns of 18, 15, 4 and 36 ng/g in sediment taken from the Scheldt estuary, Netherlands(7). 1,3-Dichlorobenzene was detected in sediment at concns of 150–300 ug/kg in Lake Ketelmeer, Netherlands(8). 1,3-Dichlorobenzene was detected in sediment off the coast of Taiwan at concns of 4–15 ng/kg(9).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

>> 1,3-Dichlorobenzene was detected at concns of 0.6, 0.6, 0.3 and 2–3 ppb in trout taken from Lake Superior, Lake Huron, Lake Erie and Lake Ontario, respectively, during 1980(1). 1,3-Dichlorobenzene was identified, not quantified, in fish caught in the Great Lakes(2).

Animal Concentrations:

Concentrations of this compound in animals.

>> 1,3-Dichlorobenzene combined with other chlorinated benzenes were identified in the blood of foxes from the Canadian Arctic(1).

Average Daily Intake:

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

>> Based on monitoring data at three USA urban sites (Los Angeles, Phoenix, Oakland), the AVDI for 1,3-dichlorobenzene has been estimated to be 0.8–1.1 ug/day(1). The AVDI (via inhalation exposure only) of combined 1,2-, 1,3- and 1,4-dichlorobenzene isomers in the Netherlands is 7.0 ug/day(2).

13. Disposal Considerations

Spillage Disposal

>> Personal protection: filter respirator for organic gases and particulates adapted to the airborne concentration of the substance. 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. Do NOT let this chemical enter the environment.

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 U071, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

>> Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number U071, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

>> ... Halogenated compounds may be disposed of by incineration provided they are blended with other compatible wastes or fuels so that the composite contains less than 30% halogens and the heating value is from 7000 to 9000 BTU/lb. Liquid injection, rotary kiln, and fluidized bed incinerators are typically used to destroy liquid halogenated wastes. ... Temperatures of at least 2000–2200 °F and residence times /of more than 2 sec/ ... are required for the destruction of halogenated aromatic hydrocarbons. /Halogenated aromatic hydrocarbons/

- >> Potential candidate for rotary kiln incineration, with a temperature range of 820 to 1,600 °C, and a residence time of seconds. Also a potential candidate for liquid injection incineration, with a temperature range of 650 to 1,600 °C, and a residence time of 0.1 to 2 seconds.
- >> For more Disposal Methods (Complete) data for 1,3-DICHLOROBENZENE (6 total), please visit the HSDB record page.

14. Transport Information

DOT

1,3-Dichlorobenzene

6.1

UN Pack Group: III

Reportable Quantity of 100 lb or 45

IATA

1,3-Dichlorobenzene

6.1,

UN Pack Group: III

15. Regulatory Information

Federal Drinking Water Standards:

Federal drinking water standards (e.g. maximum containment level (MCL)) for this chemical. These standards are legally enforceable.

- >> EPA 600 ug/l

Federal Drinking Water Guidelines:

Federal drinking water guidelines (e.g. maximum containment level (MCL)) for this chemical. In general, these guidelines are recommendations and not legally enforceable.

- >> EPA 600 ug/l

State Drinking Water Standards:

State drinking water standards (e.g. maximum containment level (MCL)) for this chemical. These standards are legally enforceable.

- >> (NJ) NEW JERSEY 600 ug/l

Clean Water Act Requirements:

The Clean Water Act (CWA) of 1972 establishes the basic structure for regulating discharges of pollutants into the waters of the United States and regulating quality standards for surface waters. Under CWA, the U.S. Environmental Protection Agency (EPA) developed the Toxic Pollutant List (40 CFR Part 401.15) and the Priority Pollutant List (40 CFR Part 423, Appendix A). These lists are to be used by EPA and States to develop the Effluent Guidelines regulations and ensure water quality criteria and standards.

- >> Toxic pollutant designated pursuant to section 307(a)(1) of the Federal Water Pollution Control Act and is subject to effluent limitations. /Dichlorobenznes (1,2-, 1,3- and 1,4-dichlorobenzenes)/

TSCA Requirements:

This section provides information on requirements concerning this chemical under the Toxic Substances Control Act (TSCA) of 1976. TSCA provides EPA with authority to require reporting, record-keeping and testing requirements, and restrictions relating to chemical substances and/or mixtures. Certain substances are generally excluded from TSCA, including, among others, food, drugs, cosmetics and pesticides.

- >> Pursuant to section 8(d) of TSCA, EPA promulgated a model Health and Safety Data Reporting Rule. The section 8(d) model rule requires manufacturers, importers, and processors of listed chemical substances and mixtures to submit to

EPA copies and lists of unpublished health and safety studies. Benzene, 1,3-dichloro- is included on this list. Effective date 10/4/82; Sunset date 10/4/92.

Regulatory Information

The Australian Inventory of Industrial Chemicals

>> Chemical: Benzene, 1,3-dichloro-

REACH Registered Substance

>> Status: Active Update: 13-03-2023 <https://echa.europa.eu/registration-dossier/-/registered-dossier/18076>

>> Status: Active Update: 07-10-2015 <https://echa.europa.eu/registration-dossier/-/registered-dossier/16616>

>> Status: Active Update: 31-03-2021 <https://echa.europa.eu/registration-dossier/-/registered-dossier/1940>

New Zealand EPA Inventory of Chemical Status

>> 1,3-Dichlorobenzene: 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 – Benzene, 1,3-dichloro-: 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."