SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : Dichlobenil
Catalog Number : io-2136
CAS Number : 1194-65-6
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)

>> Warning

GHS Hazard Statements

>> H312 (99%): Harmful in contact with skin [Warning Acute toxicity, dermal]

>> H411 (99%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

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

Health Hazards:

>> SOLID: Harmful if swallowed. (USCG, 1999)

>> Not flammable. (USCG, 1999)

>> Not combustible. Gives off irritating or toxic fumes (or gases) in a fire.

3. Composition/Information On Ingredients

Chemical name : Dichlobenil
CAS Number : 1194-65-6
Molecular Formula : C7H3Cl2N
Molecular Weight : 172.0100 g/mol

4. First Aid Measures

First Aid:

>> Call a physician.

>> EYES: Flush with water.

>> SKIN: Wash with water.

>> INGESTION: Gastric lavage and symptomatic therapy. (USCG, 1999)

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. Do NOT induce vomiting. Refer for medical attention .

5. Fire Fighting Measures

>> Not combustible. Gives off irritating or toxic fumes (or gases) in a fire.

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

>> CAUTION: Fire involving Safety devices (UN3268) and Fire suppressant dispersing devices (UN3559) may have a delayed activation and a risk of hazardous projectiles. Extinguish the fire at a safe distance.

>> SMALL FIRE: Dry chemical, CO2, water spray or regular foam.

>> LARGE FIRE: Water spray, fog or regular foam. Do not scatter spilled material with high-pressure water streams. If it can be done safely, move undamaged containers away from the area around the fire. Dike runoff from fire control for later disposal.

>> FIRE INVOLVING TANKS: 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. (ERG, 2024)

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

Storage Conditions:

>> The shelf life in storage is at least 2 yr when stored in a cool, dry place. In view of its volatility, the product should be packed in tightly closed containers.

8. Exposure Control/ Personal Protection

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 skin. This may result in chloracne.

Acceptable Daily Intakes:

An estimate of the amount of a chemical in food or drinking water that can be consumed daily over a lifetime without presenting an appreciable risk to health. It is usually expressed as milligrams of the substance per kilogram of body weight per day and applies to chemicals such as food additives, pesticide residues and veterinary drugs.

>> OPP RfD= 0.0005 mg/kg

Exposure Prevention

>> See EFFECTS OF LONG-TERM OR REPEATED EXPOSURE.

Inhalation Prevention

>> Use ventilation (not if powder), local exhaust or breathing protection.

Skin Prevention

>> Protective gloves.

Eye Prevention

>> Wear safety goggles.

Ingestion Prevention

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

Exposure Control and Personal Protection

Exposure Summary

>> TIH (Toxic Inhalation Hazard) - Term used to describe gases and volatile liquids that are toxic when inhaled. Some are TIH materials themselves, e.g., chlorine, and some release TIH gases when spilled in water, e.g., chlorosilanes. [ERG 2016].

9. Physical And Chemical Properties

Molecular Weight:

>> 172.01

Exact Mass:

>> 170.9642545

Physical Description:

>> Dichlobenil is a white solid dissolved or suspended in a water-emulsifiable liquid carrier. The primary hazard is the threat to the environment. Immediate steps should be taken to limit spread to the environment. Can easily penetrate the soil and contaminate groundwater and nearby streams. Can cause illness by inhalation, skin absorption and/or ingestion. Used as a herbicide.

>> WHITE-TO-OFF-WHITE CRYSTALS WITH CHARACTERISTIC ODOUR.

Color/Form:

>> White crystalline solid

Odor:

>> Aromatic odor

Boiling Point:

>> 518 °F at 760 mmHg (USCG, 1999)

>> 270 °C

Melting Point:

>> 293 to 294.8 °F (USCG, 1999)

>> 145-146 °C

Flash Point:

>> Not Applicable. Not flammable. (USCG, 1999)

Solubility:

>> In water, 14.6 mg/L at 20 °C

>> Solubility in water: none

Density:

>> 1.3 g/cm³

Vapor Pressure:

>> 20.94 mmHg at 220 °F (USCG, 1999)

>> Vapor pressure, Pa at 20 °C: 0.073

LogP:

>> log Kow = 2.74

>> 2.64

Stability/Shelf Life:

>> Stable to sunlight

Autoignition Temperature:

>> Not Applicable. Not flammable. (USCG, 1999)

Decomposition:

>> When heated to decomposition it emits toxic fumes of /hydrogen chloride, hydrogen cyanide, and nitrogen oxides/.

Corrosivity:

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

>> NON-CORROSIVE

10. Stability And Reactivity

>> Not soluble in water.

11. Toxicological Information

Toxicity Summary:

>> Organic nitriles decompose into cyanide ions both in vivo and in vitro. Consequently the primary mechanism of toxicity for organic nitriles is their production of toxic cyanide ions or hydrogen cyanide. Cyanide is an inhibitor of cytochrome c oxidase in the fourth complex of the electron transport chain (found in the membrane of the mitochondria of eukaryotic cells). It complexes with the ferric iron atom in this enzyme. The binding of cyanide to this cytochrome prevents transport of electrons from cytochrome c oxidase to oxygen. As a result, the electron transport chain is disrupted and the cell can no longer aerobically produce ATP for energy. Tissues that mainly depend on aerobic respiration, such as the central nervous system and the heart, are particularly affected. Cyanide is also known produce some of its toxic effects by binding to catalase, glutathione peroxidase, methemoglobin, hydroxocobalamin, phosphatase, tyrosinase, ascorbic acid oxidase, xanthine oxidase, succinic dehydrogenase, and Cu/Zn superoxide dismutase. Cyanide binds to the ferric ion of methemoglobin to form inactive cyanmethemoglobin. (L97)

EPA Human Health Benchmarks for Pesticides:

This section provides the EPA human health benchmarks non-enforceable drinking water levels related to adverse health effects from drinking water exposure to contaminants that have no drinking water standards or health advisories.

Chemical Substance

>> Dichlobenil

Acute or One Day PAD (RfD) [mg/kg/day]

>> 0.45

Acute or One Day HHBPs [ppb]

>> 13000

Acute HHBP Sensitive Lifestage/Population

>> Females 13-49 yrs

Chronic or One Day PAD (RfD) [mg/kg/day]

>> 0.01

Chronic or One Day HHBPs [ppb]

>> 60

Chronic HHBP Sensitive Lifestage/Population

>> General Population

Reference (PDF)

>> Human Health Benchmarks for Pesticides - 2021 Update

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

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

Chemical

>> Dichlobenil

USGS Parameter Code

>> 49303

Chronic Noncancer HHBP (Human Health Benchmarks for Pesticides)[µg/L]

>> 60

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).

>> 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).

>> No indication of carcinogenicity to humans (not listed by IARC).

Health Effects:

>> Exposure to high levels of cyanide for a short time harms the brain and heart and can even cause coma, seizures, apnea, cardiac arrest and death. Chronic inhalation of cyanide causes breathing difficulties, chest pain, vomiting, blood changes, headaches, and enlargement of the thyroid gland. Skin contact with cyanide salts can irritate and produce sores. (L96, L97)

Exposure Routes:

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

>> Oral (L96) ; inhalation (L96) ; dermal (L96)

Inhalation Exposure

>> Cough.

Skin Exposure

>> MAY BE ABSORBED!

Eye Exposure

>> Redness.

>> Cyanide poisoning is identified by rapid, deep breathing and shortness of breath, general weakness, giddiness, headaches, vertigo, confusion, convulsions/seizures and eventually loss of consciousness. (L96, L97)

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.

>> Dermatotoxin - Chloracne.

Toxicity Data:

>> LC50 (rat) > 3,300 mg/m3

Treatment:

Treatment when exposed to toxin

>> Antidotes to cyanide poisoning include hydroxocobalamin and sodium nitrite, which release the cyanide from the cytochrome system, and rhodanase, which is an enzyme occurring naturally in mammals that combines serum cyanide with thiosulfate, producing comparatively harmless thiocyanate. Oxygen therapy can also be administered. (L97)

Interactions:

>> Twenty-four hours following injection of a single dose of the herbicide dichlobenil (2,6-dichlorobenzonitrile) in C57Bl/6 mice a steep dose-response curve for the histopathological toxicity in the olfactory mucosa was observed. Four hours following injection of a toxic dose of [ring-14C]dichlobenil (12 mg/kg) the covalent binding in the olfactory mucosa was 26 times higher than that in the liver. A dose-dependent decrease of nonprotein sulfhydryls (mainly glutathione, GSH) in the olfactory mucosa was observed 2.5 hr following injection of dichlobenil (6, 12, 25 mg/kg). The synthetic GSH precursor N-acetyl-L-cysteine decreased both the dichlobenil-induced toxicity and the covalent binding, whereas N-acetyl-D-cysteine had no effect. No protective effects of the cyanide antidotes nitrite, thiosulfate, or superoxide dismutase on the dichlobenil-induced toxicity were observed. In mice given the GSH-depleting agent phorone and a subtoxic dose of dichlobenil (6 mg/kg), an extensive toxicity and an increased covalent binding in the olfactory mucosa were demonstrated. Autoradiography showed no change in the distribution of covalent (14)C dichlobenil binding to

nontarget tissues of phorone-treated mice. In conclusion, the results demonstrate a relationship between the degrees of covalent binding, GSH depletion, and toxicity of dichlobenil in the olfactory mucosa. Hence, the level of GSH appears to be of importance for the dichlobenil-induced toxicity in the olfactory mucosa.

Antidote and Emergency Treatment:

>> Inhalation: /get/ fresh air and rest. Skin /exposure/: Remove contaminated clothes. Rinse and then wash skin with water and soap. Eye /exposure/: first rinse with plenty of water for several minute (remove contact lenses if easily possible), then take to a doctor. Ingestion: Rinse mouth. DO NOT induce vomiting. Refer for medical attention.

Human Toxicity Excerpts:

>> /SIGNS AND SYMPTOMS/ Dichlobenil caused chloracne in six persons involved in the manufacture of Casoron. Symptoms were observed at different lag times for each individual, the longest being five months. Several hundred pinpoint open comedones and several closed comedones appeared on the forehead, masseteric, zygomatic, and suborbital regions, and occasionally an inflammatory papule or small pustule was noted. The usual forms of acne treatment did not produce improvement until the patient was withdrawn from contact with dichlobenil.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ A study was conducted to investigate whether the herbicide dichlobenil was toxic to the nasal mucosa following ip injection in mice. Microautoradiography and tape section autoradiography were used to determine the cellular targets for irreversible metabolite binding. Female C57B1 mice were given single ip injections of dichlobenil at 6, 12, 25, or 50 mg/kg. Some mice were treated with metyrapone to determine the role of cytochrome p450 in the toxicity of dichlobenil. Mice were killed at 8 hours to 20 days after treatment. Female Sprague Dawley rats were injected ip with 25 or 50 mg/kg, and killed after 3 days. Liver and nasal region tissues were fixed, sectioned, and examined histologically. Tissues from mice administered (14)C labeled dichlobenil were examined by autoradiography. The results indicated that dichlobenil is a potent olfactory toxicant that induces lesions both in the epithelium and the glands of Bowman. The herbicide is metabolized to a reactive metabolite that becomes bound in the glands. Since the binding was confined to these glands, it was proposed that there is a primary lesion in Bowman's glands and that the lesion in the olfactory epithelium is secondary.

Non-Human Toxicity Values:

>> LD50 Mouse oral male 2126 mg/kg (14 day observation period) female 2056 mg/kg (14 day observation period)

12. Ecological Information

ICSC Environmental Data:

>> The substance is toxic to aquatic organisms. 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: Dichlobenil was detected in soil of an agricultural field in Ireland at 4.55 mg/kg (2.54 cm depth) and 0.45 mg/kg (7.62-10.16 cm depth)(1).

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 sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Disposal Methods

>> SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

>> Safe Disposal of Pesticides. The best way to dispose of small amounts of excess pesticides is to use them - apply them - according to the directions on the label. If you cannot use them, ask your neighbors whether they have a similar pest control problem and can use them. If all of the remaining pesticide cannot be properly used, check with your local solid waste management authority, environmental agency, or health department to find out whether your community has a household hazardous waste collection program or a similar program for getting rid of unwanted, leftover pesticides. These authorities can also inform you of any local requirements for pesticide waste disposal.

>> Safe Disposal of Pesticides. An empty pesticide container can be as hazardous as a full one because of residues left inside. Never reuse such a container. When empty, a pesticide container should be rinsed carefully three times and the rinsewater thoroughly drained back onto the sprayer or the container previously used to mix the pesticide. Use the rinsewater as a pesticide, following label directions. Replace the cap or closure securely. Dispose of the container according to label instructions. Do not puncture or burn a pressurized container like an aerosol - it could explode. Do cut or puncture other empty pesticide containers made of metal or plastic to prevent someone from reusing them. Wrap the empty container and put it in the trash after you have rinsed it.

14. Transport Information

DOT

Dichlobenil

Reportable Quantity of 100 lb or 45

IATA

Dichlobenil

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15. Regulatory Information

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.

>> Dichlobenil is designated as a hazardous substance under section 311(b)(2)(A) of the Federal Water Pollution Control Act and further regulated by the Clean Water Act Amendments of 1977 and 1978. These regulations apply to discharges of this substance. This designation includes any isomers and hydrates, as well as any solutions and mixtures containing this substance.

Regulatory Information

REACH Registered Substance

>> Status: Active Update: 26-08-2022 https://echa.europa.eu/registration-dossier/-/registered-dossier/12680

New Zealand EPA Inventory of Chemical Status

>> Dichlobenil: 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 - Benzonitrile, 2,6-dichloro-: Environment tier I assessment

>> IMAP assessments - Benzonitrile, 2,6-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."