SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : 2,2-Dichloropropionic acid
Catalog Number : io-2191
CAS Number : 75-99-0
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 (10.4%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H315 (100%): Causes skin irritation [Warning Skin corrosion/irritation]

>> H318 (100%): Causes serious eye damage [Danger Serious eye damage/eye irritation]

>> H412 (100%): Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P264, P264+P265, P270, P273, P280, P301+P317, P302+P352, P305+P354+P338, P317, P321, P330, P332+P317, P362+P364, and P501

Health Hazards:

>> VAPOR: Irritating to eyes, nose and throat. LIQUID: Will burn skin and eyes. Harmful if swallowed. (USCG, 1999)

>> Combustible. Irritating fumes of hydrochloric acid may form in fire. Volatilizes with steam. (USCG, 1999)

>> Gives off irritating or toxic fumes (or gases) in a fire.

3. Composition/Information On Ingredients

Chemical name : 2,2-Dichloropropionic acid
CAS Number : 75-99-0
Molecular Formula : C3H4Cl2O2
Molecular Weight : 142.9700 g/mol

4. First Aid Measures

First Aid:

>> Excerpt from NIOSH Pocket Guide for 2,2-Dichloropropionic acid:

>> Eye: IRRIGATE IMMEDIATELY - If this chemical contacts the eyes, immediately wash (irrigate) the eyes with large amounts of water, occasionally lifting the lower and upper lids. Get medical attention immediately.

>> Skin: WATER WASH IMMEDIATELY - If this chemical contacts the skin, immediately wash the contaminated skin with water. If this chemical penetrates the clothing, immediately remove the clothing and wash the skin with water. If symptoms occur after washing, get medical attention immediately.

>> Breathing: RESPIRATORY SUPPORT - If a person breathes large amounts of this chemical, move the exposed person to fresh air at once. If breathing has stopped, perform artificial respiration. Keep the affected person warm and at rest. Get medical attention as soon as possible.

>> Swallow: MEDICAL ATTENTION IMMEDIATELY - If this chemical has been swallowed, get medical attention immediately. (NIOSH, 2024)

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.

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

>> Give one or two glasses of water to drink. Do NOT induce vomiting. Refer for medical attention .

5. Fire Fighting Measures

>> Irritating fumes may form in fire. Volatilizes with steam.

>> Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]:

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

>> LARGE FIRE: Dry chemical, CO2, alcohol-resistant foam or water spray. 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, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Do not get water inside containers. 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)

>> 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 154 [Substances - Toxic and/or Corrosive (Non-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: particulate filter respirator adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. If liquid: collect leaking liquid in sealable containers as far as possible. If solid: sweep spilled substance into containers. Carefully collect remainder. Then store and dispose of according to local regulations.

7. Handling And Storage

Safe Storage:

>> Separated from food and feedstuffs. Dry. Well closed.

Storage Conditions:

>> Keep container tightly closed when not in use.

8. Exposure Control/ Personal Protection

REL-TWA (Time Weighted Average)

>> 1 ppm (6 mg/m³)

>> TWA 1 ppm (6 mg/m3)

>> none See Appendix G

>> 5.0 [mg/m3], inhalable fraction

>> (inhalable fraction): 5 mg/m

TLV-TWA (Time Weighted Average)

>> 5 mg/m³ (inhalable particulate matter) [1997]

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 substance is irritating to the eyes, skin and respiratory tract.

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= 0.03 mg/kg; EPA RfD= 0.03 mg/kg

Inhalation Prevention

>> Use ventilation, local exhaust or breathing protection.

Skin Prevention

>> Protective gloves.

Eye Prevention

>> Wear safety goggles or eye protection in combination with breathing protection.

Ingestion Prevention

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

9. Physical And Chemical Properties

Molecular Weight:

>> 142.97

Exact Mass:

>> 141.9588348

Physical Description:

>> 2,2-dichloropropionic acid appears as a colorless liquid. Soluble in water. Corrosive to metals and tissue. Used as a herbicide.

>> HYGROSCOPIC WHITE SOLID IN VARIOUS FORMS OR COLOURLESS LIQUID.

Color/Form:

>> Liquid

Odor:

>> Acrid odor.

Boiling Point:

>> 374 °F at 760 mmHg (USCG, 1999)

>> 190 °C

Melting Point:

>> 46 °F (USCG, 1999)

>> 20 °C

Solubility:

>> 50 % (NIOSH, 2024)

>> Solubility in water, g/100ml at 25 °C: 90

Density:

>> 1.4 (NIOSH, 2024) - Denser than water; will sink

>> Relative density (water = 1): 1.40

Vapor Density:

>> 4.9 (USCG, 1999) - Heavier than air; will sink (Relative to Air)

Vapor Pressure:

>> 5.07 mmHg at 160 °F (USCG, 1999)

LogP:

>> log Kow= 0.78

>> 0.76

Stability/Shelf Life:

>> Subject to hydrolysis; slight at 25 °C, but comparatively rapid >/=50 °C; so aqueous solutions should not be kept for any length of time. Alkali causes dehydrochlorination above 120 °C.

Decomposition:

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

Corrosivity:

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

>> Corrosive to iron

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.

>> (Aq): 1.32 (0.099 N, 23 °C)

Odor Threshold:

>> 2,500 mg/cu m

Refractive Index:

>> Index of refraction: 1.4551 @ 20 °C

Dissociation Constants:

>> pKa average = 1.74 at 0.001 to 0.1 molarity of the acid and 1.84 at 0.05 ionic strength

10. Stability And Reactivity

>> Soluble in water. Reacts slowly in water to form hydrochloric and pyruvic acids.

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).

>> A4; Not classifiable as a human carcinogen.

Exposure Routes:

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

>> inhalation, ingestion, skin and/or eye contact

Inhalation Exposure

>> Burning sensation. Cough. Sore throat.

Skin Exposure

>> Redness. Pain.

Eye Exposure

>> Redness. Pain. Blurred vision.

Ingestion Exposure

>> Burning sensation. Diarrhoea. Nausea. Vomiting.

>> irritation eyes, skin, upper respiratory system; skin burns; lassitude (weakness, exhaustion), loss of appetite, diarrhea, vomiting, slowing of pulse; central nervous system depression

Target Organs:

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

>> Urinary

>> Eyes, skin, respiratory system, gastrointestinal tract, central nervous system

Adverse Effects:

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

>> Dermatotoxin - Skin burns.

>> ACGIH Carcinogen - Not Classifiable.

Interactions:

>> Investigation of several derivatives ... has failed to reveal any with greater biological activity than sodium salt. ... Activity ... enhanced by changing pH or by adding any of several suitable surfactants. Latter alters physiologically important ionic & polar properties of dalapon solution.

Antidote and Emergency Treatment:

>> Treatment is symptomatic and supportive. Oils should not be used as either cathartics or dermal cleansing agents, as they increase absorption. Gastric lavage and use of activated charcoal and sodium sulfate are indicated for ingestion. If dermal exposure occurred, contaminated clothes should be removed, and the skin should be thoroughly cleansed with soap and water. Management of seizures in both children and adults is with Valium or phenobarbital. Respiratory depression and even respiratory arrest, especially with concomitant use of Valium and phenobarbital in children, may occur. These drugs preferably should be used only in critical care areas where emergency endotracheal intubation can be performed. /It is recommended/ that epinephrine not be utilized in patients with organochlorine poisoning, as the organochlorines induce myocardial irritability and ventricular arrhythmias may occur. However, dopamine may be necessary in the event of hypotension unresponsive to fluid administration, and epinephrine may be necessary in the event of cardiopulmonary arrest. /Organochlorine insecticides/

Human Toxicity Excerpts:

>> /SIGNS AND SYMPTOMS/ ...Repeated, prolonged /skin/ contact /may cause/ a mild burn. Eyes ... transient corneal injury.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ ... /Rainbow trout fry (Salmo gairdneri)/ avoided copper sulfate (0.0001 mg/l), dalapon (1.0 mg/l), 2,4-D, (1.0 mg/l), xylene (0.1 mg/l), and acrolein (0.1 mg/l), but did not avoid glyphosate, Aquathol K, or diquat at concentrations below 10 mg/l or TCA at concentrations less than 1.0 mg/l.

Non-Human Toxicity Values:

>> LD50 Rat (male) oral 7126 mg/kg

12. Ecological Information

Resident Soil (mg/kg)

>> 1.90e+03

Industrial Soil (mg/kg)

>> 2.50e+04

Tapwater (ug/L)

>> 6.00e+02

MCL (ug/L)

>> 2.00e+02

Risk-based SSL (mg/kg)

>> 1.20e-01

MCL-based SSL (mg/kg)

>> 4.10e-02

Chronic Oral Reference Dose (mg/kg-day)

>> 3.00e-02

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Fraction of Contaminant Absorbed Dermally from Soil

>> 0.1

ICSC Environmental Data:

>> The substance is harmful to aquatic organisms.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> ... In one soil, 2,660 ppm dalapon significantly increased production of ammonium-nitrogen; nitrification was almost totally inhibited in this soil.

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. If liquid: collect leaking liquid in sealable containers as far as possible. If solid: sweep spilled substance into containers. 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.

>> Dalapon-sodium can be incinerated in a unit with effluent gas scrubbing. Recommendable methods: Incineration, alkaline hydrolysis. /Dalapon sodium/

14. Transport Information

DOT

2,2-Dichloropropionic acid

Reportable Quantity of 5,000 lb or 2,270 kg

IATA

2,2-Dichloropropionic acid

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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 200 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 200 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.

>> 2,2-Dichloropropionic acid 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

New Zealand EPA Inventory of Chemical Status

>> Dalapon: 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 - Propanoic acid, 2,2-dichloro-: Environment tier I assessment

>> IMAP assessments - Propanoic acid, 2,2-dichloro-: Human health tier I assessment

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