SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : 3,6-Dichloro-2-methoxybenzoic acid
Catalog Number : io-2164
CAS Number : 1918-00-9
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+H332 (14.2%): Harmful if swallowed or if inhaled [Warning Acute toxicity, oral; acute toxicity, inhalation]

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

>> H318 (99.7%): Causes serious eye damage [Danger Serious eye damage/eye irritation]

>> H332 (56.9%): Harmful if inhaled [Warning Acute toxicity, inhalation]

>> H335 (30.6%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]

>> H400 (26.4%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]

>> H410 (26.4%): Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]

>> H412 (99.3%): Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P261, P264, P264+P265, P270, P271, P273, P280, P301+P317, P304+P340, P305+P354+P338, P317, P319, P330, P391, P403+P233, P405, and P501

Health Hazards:

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

>> Not flammable. (USCG, 1999)

>> Not combustible. 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 : 3,6-Dichloro-2-methoxybenzoic acid
CAS Number : 1918-00-9
Molecular Formula : C8H6Cl2O3
Molecular Weight : 221.0300 g/mol

4. First Aid Measures

First Aid:

>> EYES: Flush with water; obtain medical attention.

>> SKIN: Wash with ample water.

>> INGESTION: Induce vomiting. (USCG, 1999)

First Aid Measures

Inhalation First Aid

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

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. Refer for medical attention .

5. Fire Fighting Measures

>> Liquid formulations containing organic solvents may be flammable.

>> 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 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:

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

Storage Conditions:

>> Keep container tightly closed in a dry and well-ventilated place.

8. Exposure Control/ Personal Protection

Inhalation Risk:

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

Effects of Short Term Exposure:

>> The substance is severely irritating to the eyes. The substance is irritating to the 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

Exposure Prevention

>> PREVENT DISPERSION OF DUST! AVOID EXPOSURE OF ADOLESCENTS AND CHILDREN!

Inhalation Prevention

>> Use 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.

9. Physical And Chemical Properties

Molecular Weight:

>> 221.03

Exact Mass:

>> 219.9693994

Physical Description:

>> Dicamba is a white solid dissolved in a liquid carrier. The carrier is water emulsifiable. The primary hazard is the threat to the environment. Immediate steps should be taken to limit its spread to the environment. Since it is a liquid it can easily penetrate the soil and contaminate groundwater and nearby streams. It can cause illness by inhalation, skin absorption and/or ingestion. It is used as a herbicide.

>> COLOURLESS CRYSTALS.

Color/Form:

>> Crystals from pentane

Odor:

>> Odorless (reference grade)

Boiling Point:

>> > 200 °C

Melting Point:

>> 237.2 to 240.8 °F (USCG, 1999)

>> 114-116 °C

Flash Point:

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

Solubility:

>> In water, 8310 mg/L at 25 °C

>> Solubility in water, g/100ml at 25 °C: 0.79

Density:

>> 1.57 g/cu cm at 25 °C

>> Relative density (water = 1): 1.57

Vapor Density:

>> 7.62 (USCG, 1999) - Heavier than air; will sink (Relative to Air)

Vapor Pressure:

>> 0.0000338 [mmHg]

>> Vapor pressure, Pa at 25 °C: 0.0045

LogP:

>> log Kow = 2.21

>> 2.21

Stability/Shelf Life:

>> Stable under recommended storage conditions.

Autoignition Temperature:

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

Decomposition:

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

>> 200 °C

Corrosivity:

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

>> Mild to noncorrosive

Odor Threshold:

>> /SRP: Air/ 250.8 PPM

Dissociation Constants:

>> pKa = 1.97

Collision Cross Section:

Collision cross section (CCS) represents the effective area for the interaction between an individual ion and the neutral gas through which it is traveling (e.g., in ion mobility spectrometry (IMS) experiments). It quantifies the probability of a collision taking place between two or more particles.

>> 157.21 Å² [M+Na]+ [CCS Type: DT; Method: stepped-field]

10. Stability And Reactivity

>> No rapid reaction with air. No rapid reaction with water.

11. Toxicological Information

Toxicity Summary:

>> IDENTIFICATION AND USE: Dicamba is a crystalline solid, white (reference grade) or brown (technical grade). It is a growth regulating herbicide. It controls broadleaf weeds in asparagus, corn (field, silage, popcorn), grass seed crops, grain sorghum, noncropland, pastures, rangeland, reduced-tillage, fallow, small grains not underseeded to legumes, sugarcane, turf, between cropping; brush and vines in pastures, industrial areas, noncropland, rangeland; perennial broadleaf weeds with spot treatments and ropewick applications. HUMAN STUDIES: Dicamba is moderately toxic by ingestion and slightly toxic by inhalation or dermal exposure. Symptoms of poisoning with dicamba include loss of appetite (anorexia), vomiting, muscle weakness, slowed heart rate, shortness of breath, central nervous system effects (victim may become excited or depressed), benzoic acid in the urine, incontinence, cyanosis (bluing of the skin and gums), and exhaustion following repeated muscle spasms. In addition to these symptoms, inhalation can cause irritation of the linings of the nasal passages and the lungs, and loss of voice. Most individuals who have survived severe poisoning from dicamba have recovered within 2 to 3 days with no permanent effects. Dicamba is capable of inducing DNA damage since it significantly increases the unwinding rate for liver DNA in vivo and also induces unscheduled DNA synthesis in human peripheral blood lymphocytes in vitro in the presence of exogenous metabolic activation. Furthermore, dicamba causes a very slight increase in sister chromatid exchange frequency in human peripheral blood lymphocytes in vitro. ANIMAL STUDIES: In rabbits, dose-related dermal irritation was observed. Desquamation was seen predominantly in the 1000 mg/kg/day group while moderate erythema, moderate edema and atonia were observed exclusively in the 1000 mg/kg/day group. Technical dicamba was fed in diet to rats (60/sex/group) at 0, 50, 250 or 2500 ppm in the diet for 115 to 118 weeks. Brain ventricular dilatation associated with pituitary anterior adenomas were observed in females at >/= 250 ppm. Adrenal enlargement was increased at >/= 250 ppm in both sexes. Increased macroscopic lesions in liver at >/= 250 ppm (males) and lesions in lymph nodes at 2500 ppm (males) were observed. There were increased malignant lymphomas in females at >/= 250 ppm, increased parafollicular cell carcinoma, and adenoma, as well as increased follicular adenoma and carcinomas in treated males, primarily at 2500 ppm, but could be extended down to the lower doses. Chronic treatment of adult and newborn rats with less than 0.04xLD50 of dicamba caused disorder of oxidative phosphorylation and focal necrosis in the heart. Similar changes were observed in rat embryos of dams exposed to the pesticide. In a rat developmental study, no treatment-related fetotoxicity or developmental effects were observed at any dose level based on assessments of numbers of pregnancies, implantation and resorption sites, and viable and dead fetuses, as well as litter weights and external, skeletal and visceral fetal examinations. Dicamba was negative in the Ames test with Salmonella typhimurium TA98, TA100, TA1535, TA1537 and

TA102 with or without activation. ECOTOXICITY STUDIES: In fish, dicamba exposure could result in histological lesions, plasma vitellogenin increases, changes in sex hormone levels, and alterations of hormone-related gene expression. Dicamba induced primary DNA breaks in amphibians. Dicamba significantly increased lady beetle mortality and reduced their body weight. Plants exposed to sublethal levels of dicamba may produce fewer floral resources and be less frequently visited by pollinators.

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

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

Chemical

>> Dicamba

USGS Parameter Code

>> 68571

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

>> 200

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 D Not Classifiable as to Human Carcinogenicity

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:

>> In oral, dermal, and inhaled routes of exposure, dicamba has a low acute toxicity. Dicamba may have irritating or corrosive effects on the skin and eyes. The EPA has identified dicamba as a developmental toxin in the Toxics Release Inventory. (L2156)

Exposure Routes:

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

>> Oral; inhalation; dermal

Inhalation Exposure

>> Cough. Sore throat.

Skin Exposure

>> Redness. Pain.

Eye Exposure

>> Redness. Pain. Blurred vision.

Ingestion Exposure

>> Nausea. Vomiting. Weakness. Convulsions.

>> Exposing the skin and eyes to dicamba can cause redness, pain, and blurred vision. The inhalation of dicamba may cause coughing, labored breathing, vomiting, and weakness. Nausea and convulsions may also result from ingestion. (L2156)

Target Organs:

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

>> Developmental

Adverse Effects:

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

>> Neurotoxin - Other CNS neurotoxin

>> Dermatotoxin - Skin burns.

Toxicity Data:

>> oral LD50 in rats: 757 mg/kg body weight, dermal LD50 in rats: >2,000 mg/kg, inhalation LC50 in rats: >200 mg/L (L371)

Treatment:

Treatment when exposed to toxin

>> Treatment may include washing any areas of contact, GI decontamination if swallowed, administering an IV and forced alkaline diuresis. (L346)

Interactions:

>> ... Pretreatment of wild garlic (Allium vineale L) shoots with low concentration of 2-chloroethylphosphonic acid ... increased basipetal translocation of foliar-applied dicamba. Pretreatment of excised bean leaves with endothall (7-oxabicylo-(2,2,1)heptane-2,3-dicarboxylic acid) greatly reduced subsequent dicamba vein loading and transport. Polar transport was activated by ATP and inhibited by 2,4-dinitrophenol (DNP). Dicamba uptake and retention were increased either by addition of 2% sucrose or by prior exposure of plants to sunlight.

Antidote and Emergency Treatment:

>> 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. /Chlorophenoxy Herbicides and Related Compounds/

Human Toxicity Excerpts:

>> /SIGNS AND SYMPTOMS/ Despite a widespread use of dicamba herbicide and numerous animal model studies, there had not been studies on acute toxicity of this chemical compound in human subjects following ingestion. Therefore, this study was conducted to investigate clinical characteristics of dicamba poisoning and to guide physicians treating patients intoxicated with dicamba herbicide. A retrospective observational case series was conducted for 14 patients with history of dicamba herbicide ingestion. Data were collected for clinical manifestation, patient management, and final outcome. The most common symptom was altered mental state (Glasgow Coma Scale </= 14). Laboratory abnormalities were elevations in lactate, and creatine kinase, metabolic acidosis (pH < 7.35, and HCO3(-) < 20 mmol/L), and elevated lipase. QTc prolongation was commonly observed. These abnormal clinical findings had normalized within two days of supportive treatment after dicamba ingestion. One patient did demonstrate corrosive esophagitis. Acute toxicity of dicamba herbicide in human following oral exposure was manageable with supportive treatment. However, physician should take into account for corrosive effect on GI tract, rhabdomyolysis, or acute pancreatitis.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ In histopathological studies, cellular alterations in lungs, liver, kidney, adrenal gland and spleen were found. ... /Dicamba dimethyl amine salt/

Non-Human Toxicity Values:

>> LD50 Rat oral 2,740 mg/kg

Populations at Special Risk:

>> The use of pesticides has enhanced the health and economies of nations around the world by improving crop production. However, pesticides may pose health risks, particularly to the fetus and young children. In a secondary analysis of the Ontario Farm Family Health Study, we explored the relationship between birth defects and parental pesticide exposure during the 3 months prior to conception and the first trimester of pregnancy. A total of 3412 pregnancies were included in the study. Logistic regression fit by maximum likelihood was used in the analysis. The results showed that pre-conception exposure to both cyanazine (odds ratio=4.99, 95% confidence interval: 1.63-15.27) and dicamba (OR=2.42, 95% CI: 1.06-5.53) were associated with increased risk of birth defects in male offspring. Nevertheless, given the self-reported nature of the exposure and outcomes in this study, the present findings should be considered primarily as hypothesis generating, requiring verification in subsequent investigations.

12. Ecological Information

Resident Soil (mg/kg)

>> 1.90e+03

Industrial Soil (mg/kg)

>> 2.50e+04

Tapwater (ug/L)

>> 5.70e+02

MCL (ug/L)

>> 5.00e-02

Risk-based SSL (mg/kg)

>> 1.50e-01

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. 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: In soil samples collected in 2005 from Abbotsford, Bratts Lake, St Anicet, Baie St Francois and Kensington, Canada, dicamba was not detected (detection limit 0.1 ng/g)(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 containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Disposal Methods

>> SRP: 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 air, soil or water; effects on animal, aquatic and plant life; and conformance with environmental and public health regulations. If it is possible or reasonable use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination.

>> SRP: Wastewater from contaminant suppression, cleaning of protective clothing/equipment, or contaminated sites should be contained and evaluated for subject chemical or decomposition product concentrations. Concentrations shall be lower than applicable environmental discharge or disposal criteria. Alternatively, pretreatment and/or discharge to a permitted wastewater treatment facility is acceptable only after review by the governing authority and assurance that "pass through" violations will not occur. Due consideration shall be given to remediation worker exposure (inhalation, dermal and ingestion) as well as fate during treatment, transfer and disposal. If it is not practicable to manage the chemical in this fashion, it must be evaluated in accordance with EPA 40 CFR Part 261, specifically Subpart B, in order to determine the appropriate local, state and federal requirements for disposal.

>> Product: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Contaminated packaging: Dispose of as unused product.

>> Do not discharge effluent containing this product into lakes, streams, ponds, estuaries, oceans, or other waters unless in accordance with the requirements of a National Pollution Discharge Elimination System (NPDES) permit and the permitting authority has been notified in writing prior to discharge. ... For guidance contact your State Water Board or Regional Office of the EPA.

>> For more Disposal Methods (Complete) data for Dicamba (9 total), please visit the HSDB record page.

14. Transport Information

DOT

3,6-Dichloro-2-methoxybenzoic acid

Reportable Quantity of 1,000 lb or 454 kg

IATA

3,6-Dichloro-2-methoxybenzoic acid

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15. Regulatory Information

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 400 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.

>> Dicamba 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

>> Dicamba acid: HSNO Approval: HSR003321 Approved with controls

16. Other Information

Toxic Combustion Products:

Toxic products (e.g., gases and vapors) produced from the combustion of this chemical.

>> Special hazards arising from the substance or mixture: Carbon oxides, hydrogen chloride gas.

Other Safety Information

Chemical Assessment

>> IMAP assessments - Benzoic acid, 3,6-dichloro-2-methoxy-: Human health tier I assessment

>> IMAP assessments - Benzoic acid, 3,6-dichloro-2-methoxy-: Environment 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."