ionz

SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : 4,6-Dinitro-o-cresol and salts
Catalog Number : io-2267
CAS Number : 534-52-1
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)

GHS Hazard Statements

>> H300+H310+H330 (70.7%): Fatal if swallowed, in contact with skin or if inhaled [Danger Acute toxicity, oral; acute toxicity, dermal; acute toxicity, inhalation]

>> H300 (100%): Fatal if swallowed [Danger Acute toxicity, oral]

>> H310 (100%): Fatal in contact with skin [Danger Acute toxicity, dermal]

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

>> H317 (100%): May cause an allergic skin reaction [Warning Sensitization, Skin]

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

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

>> H341 (100%): Suspected of causing genetic defects [Warning Germ cell mutagenicity]

>> H400 (97.6%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]

>> H410 (100%): Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P203, P260, P261, P262, P264, P264+P265, P270, P271, P272, P273, P280, P284, P301+P316, P302+P352, P304+P340, P305+P354+P338, P316, P317, P318, P320, P321, P330, P332+P317, P333+P317, P361+P364, P362+P364, P391, P403+P233, P405, and P501

Health Hazards:

>> Extremely toxic material; probable oral lethal dose is 5-50 mg/kg in humans or between 7 drops and 1 teaspoonful for a 70 kg (150 lb.) person. (EPA, 1998)

>> Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

>> Combustible material: may burn but does not ignite readily. When heated, vapors may form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Corrosives in contact with metals may evolve flammable hydrogen gas. Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a molten form. (ERG, 2024)

>> Combustible. Gives off irritating or toxic fumes (or gases) in a fire. Finely dispersed particles form explosive mixtures in air. Risk of fire and explosion on contact with oxidizing agents.

3. Composition/Information On Ingredients

Chemical name : 4,6-Dinitro-o-cresol and salts
CAS Number : 534-52-1
Molecular Formula : C7H6N2O5
Molecular Weight : 198.1300 g/mol

4. First Aid Measures

First Aid:

>> Warning: Effects may be delayed for several hours. Toxicity of dinitrocresol is enhanced by high ambient temperature and physical activity. Caution is advised.

>> Signs and Symptoms of Acute Dinitrocresol Exposure: Early manifestations of acute dinitrocresol exposure include fever, sweating, headache, and confusion. Blood pressure, pulse, and respiratory rate are often elevated. Severe exposure may result in restlessness, seizures, and coma. Other signs and symptoms include dyspnea (shortness of breath), cyanosis (blue tint to skin and mucous membranes), pulmonary edema, nausea, vomiting, and abdominal pain. Liver injury with associated jaundice, kidney failure, and cardiac arrhythmias are commonly noted. Dermal exposure results in yellow staining of the skin and may produce burns. Dinitrocresol may irritate and burn the eyes and mucous membranes.

>> Emergency Life-Support Procedures: Acute exposure to dinitrocresol may require decontamination and life support for the victims. Emergency personnel should wear protective clothing appropriate to the type and degree of contamination. Air-purifying or supplied-air respiratory equipment should also be worn, as necessary. Rescue vehicles should carry supplies such as plastic sheeting and disposable plastic bags to assist in preventing spread of contamination.

>> Inhalation Exposure:

>> 1. Move victims to fresh air. Emergency personnel should avoid self-exposure to dinitrocresol.

>> 2. Evaluate vital signs including pulse and respiratory rate, and note any trauma. If no pulse is detected, provide CPR. If not breathing, provide artificial respiration. If breathing is labored, administer oxygen or other respiratory support.

>> 3. Obtain authorization and/or further instructions from the local hospital for administration of an antidote or performance of other invasive procedures.

>> 4. RUSH to a health care facility.

>> Dermal/Eye Exposure:

>> 1. Remove victims from exposure. Emergency personnel should avoid self- exposure to dinitrocresol.

>> 3. Remove contaminated clothing as soon as possible.

>> 4. If eye exposure has occurred, eyes must be flushed with lukewarm water for at least 15 minutes.

>> 5. Wash exposed skin areas twice with soap and water.

>> 6. Obtain authorization and/or further instructions from the local hospital for administration of an antidote or performance of other invasive procedures.

>> 7. RUSH to a health care facility.

>> Ingestion Exposure:

>> 1. Evaluate vital signs including pulse and respiratory rate, and note any trauma. If no pulse is detected, provide CPR. If not breathing, provide artificial respiration. If breathing is labored, administer oxygen or other respiratory support.

>> 2. Obtain authorization and/or further instructions from the local hospital for administration of an antidote or performance of other invasive procedures.

>> 3. DO NOT induce vomiting.

>> 4. Give the victims water or milk: children up to 1 year old, 125 mL (4 oz or 1/2 cup); children 1 to 12 years old, 200 mL (6 oz or 3/4 cup); adults, 250 mL (8 oz or 1 cup). Water or milk should be given only if victims are conscious and alert.

>> 5. Activated charcoal may be administered if victims are conscious and alert. Use 15 to 30 g (1/2 to 1 oz) for children, 50 to 100 g (1-3/4 to 3-1/2 oz) for adults, with 125 to 250 mL (1/2 to 1 cup) of water.

>> 6. Promote excretion by administering a saline cathartic or sorbitol to conscious and alert victims. Children require 15 to 30 g (1/2 to 1 oz) of cathartic; 50 to 100 g (1-3/4 to 3-1/2 oz) is recommended for adults.

>> 7. RUSH to a health care facility. (EPA, 1998)

First Aid Measures

Inhalation First Aid

>> Fresh air, rest. Artificial respiration may be needed. 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. Give a slurry of activated charcoal in water to drink. Refer for medical attention .

5. Fire Fighting Measures

>> Keep unnecessary people away; isolate hazard area. Stay upwind and keep out of low areas. Wear self-contained breathing apparatus and full protective clothing. Move container from fire area if you can do so without risk.

>> Extinguish fire with water, foam, dry chemical, carbon dioxide. (EPA, 1998)

>> Use water spray, foam, dry powder, 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: chemical protection suit including self-contained breathing apparatus. 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:

>> Separated from strong oxidants and food and feedstuffs. Well closed.

Storage Conditions:

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

8. Exposure Control/ Personal Protection

>> TWA 0.2 mg/m3 [skin]

>> 0.2 [mg/m3]

>> 0.2 [mg/m3], inhalable fraction and vapor

>> (inhalable fraction and vapour): 0.2 mg/m

MAK (Maximale Arbeitsplatz Konzentration)

>> (vapour and aerosol): skin absorption (H)

Inhalation Risk:

>> A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance at 20 °C; on spraying or dispersing, however, much faster.

Effects of Short Term Exposure:

>> The substance is corrosive to the eyes. The substance is irritating to the skin. The substance may cause effects on the metabolic rate. Exposure at high levels could cause death.

Fire Prevention

>> NO open flames. NO contact with oxidizing agents. Closed system, dust explosion-proof electrical equipment and lighting. Prevent deposition of dust.

Exposure Prevention

>> PREVENT DISPERSION OF DUST! STRICT HYGIENE!

Inhalation Prevention

>> Use local exhaust or breathing protection.

Skin Prevention

>> Protective gloves. Protective clothing.

Eye Prevention

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

Ingestion Prevention

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

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:

>> 198.13

Exact Mass:

>> 198.02767130

Physical Description:

>> 4,6-dinitro-o-cresol appears as a yellow solid. Emits toxic oxides of nitrogen fumes when heated to decomposition. Toxic by skin absorption, inhalation or ingestion. Soluble in alcohol, acetone, ether and solutions of sodium or potassium hydroxides.

>> ODOURLESS YELLOW CRYSTALS.

Color/Form:

>> Yellow prisms or needles from alcohol

Odor:

>> Odorless

Boiling Point:

>> 594 °F at 760 mmHg (EPA, 1998)

>> 312 °C

Melting Point:

>> 190 °F (NIOSH, 2024)

>> 87.5 °C

Flash Point:

>> None (EPA, 1998)

Solubility:

>> 0.01 % (NIOSH, 2024)

>> Solubility in water, g/100ml at 20 °C: 0.694

Density:

>> greater than 1.1 at 68 °F (est) (USCG, 1999)

>> 1.58 g/cm³

Vapor Density:

>> 6.82 (EPA, 1998) - Heavier than air; will sink (Relative to Air)

>> Relative vapor density (air = 1): 6.8

Vapor Pressure:

>> 5e-05 mmHg (EPA, 1998)

>> Vapor pressure, Pa at 25 °C: 0.016

LogP:

>> log Kow = 2.13

>> 2.56

Stability/Shelf Life:

>> Stable under recommended storage conditions.

Autoignition Temperature:

>> 340 °C

Decomposition:

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

Heat of Combustion:

>> -7,050 Btu/lb = -3920 cal/g = -164X10+5 J/kg

Dissociation Constants:

>> pKa = 4.31

10. Stability And Reactivity

>> Slightly soluble in water.

11. Toxicological Information

Toxicity Summary:

>> IDENTIFICATION: 4,6-Dinitro-ortho-cresol (DNOC) is a yellow crystalline solid. It is partly soluble in water. DNOC was fungicide, herbicide and insecticide that is no longer registered for use in the U.S. HUMAN STUDIES: Symptoms of DNOC toxicity include restlessness, a sensation of heat, flushed skin, sweating, thirst and deep rapid respiration and tachycardia, severe increase in body temperature, cyanosis leading to collapse, coma and death. Effects are enhanced at high temperatures. Cardiovascular effects have been noted secondary to cellular anoxia but do not appear to be consistent cardinal signs of DNOC exposure in humans. Elevated pulse rates, tachycardia, and palpitations were observed in several patients. Negative results were found in human lymphocytes for sister chromatid exchanges and unscheduled DNA synthesis in both the presence and the absence of metabolic activation at doses up to 50 ug/mL. ANIMAL STUDIES: Dietary administration of DNOC for up to 90 days decreased body weight gain in rats, mice and dogs, usually without significant alteration in food consumption. At high doses, the liver is affected , as shown by an increased activity of liver enzymes. Blood urea levels were also increased at high doses. Environmental temperatures influenced the mortality rate among rats orally dosed with DNOC. Six of 12 rats died after receiving 20 mg/kg at 37-40 °C, while only 2 of 12 rats died after receiving twice the dose (40 mg/kg) at 20-22 °C. Application of DNOC to skin of rabbits induced edema. It was a skin sensitizer in the guinea pig and corrosive to the eyes of the rabbit. Diets containing 0.25% DNOC (or 2500 mg/kg feed) were administered for 2 days to 5-day-old white Peking ducklings. Cataracts were produced within 24 hr in all the birds. This concentration induced 56% mortality the first day and 100% the second day. At high doses, DNOC has a slight effect on reproduction in the form of reduction of body weight and litter size. Other reproduction parameters were not affected. DNOC did not induce any teratogenic effects in pregnant rats receiving oral doses from gestation day 6 to day 15. In rabbits treated orally, the high dose was maternally toxic, inducing mortality. At this high dose level, teratogenic effects included microphthalmia and hydroencephaly or microencephaly. Pregnant rabbits exposed to a cutaneous application of DNOC during gestation, induced maternal toxicity at a high dose resulting in some embryotoxicity but not teratogenicity. No evidence of teratogenicity or embryotoxicity were noted in mice treated orally or by ip administration during pregnancy. DNOC has been shown to have mutagenic potential in bacterial mutagenicity systems (strains TA98 and TA100) both in the presence and absence of metabolic activation. The mutagenic response obtained in the Ames test was markedly reduced or abolished when the nitroreductase strains TA98NR and TA100NR were used, indicating involvement of nitroreductase. ECOTOXICITY STUDIES: DNOC has little effect on soil microorganisms. Acute toxicity to aquatic organisms is variable. Fish were the most sensitive species in laboratory tests. DNOC is acutely toxic for birds, mammals and honeybees.

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

>> 4,6-Dinitro-o-cresol

Reference Dose (RfD), Subchronic

>> 8 x 10^-4 mg/kg-day

PPRTV Assessment

>> PDF Document

Weight-Of-Evidence (WOE)

>> Inadequate information to assess carcinogenic potential

Last Revision

>> 2010

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

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

Chemical

>> 4,6-Dinitro-2-methylphenol

Reference

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

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 DNOC may cause mild damage to the stomach, kidneys, and liver. Ingesting DNOC for long periods may cause cataracts and skin rashes. (L198)

Exposure Routes:

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

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

Inhalation Exposure

>> Sweating. Fever. Nausea. Shortness of breath. Laboured breathing. Headache. Convulsions. Unconsciousness.

Skin Exposure

>> MAY BE ABSORBED! Yellow staining of the skin. Further see Inhalation.

Eye Exposure

>> Redness. Pain.

Ingestion Exposure

>> Abdominal pain. Vomiting. Further see Inhalation.

>> Sense of well being; headache, fever, lassitude (weakness, exhaustion), profuse sweating, excess thirst, tachycardia, hyperpnea, cough, short breath, coma

Target Organs:

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

>> Cardiovascular (Heart and Blood Vessels), Immunological (Immune System), Neurological (Nervous System)

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.

>> Nephrotoxin - The chemical is potentially toxic to the kidneys in the occupational setting.

>> Methemoglobinemia - The presence of increased methemoglobin in the blood; the compound is classified as secondary toxic effect

>> Other Poison - Uncoupler

Toxicity Data:

>> LCLo (cats) = 40 mg/m3/4 hr

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. /Phenols and related compounds/

Human Toxicity Excerpts:

>> /HUMAN EXPOSURE STUDIES/ Single oral dose of 75 mg produced no toxic effect in 5 volunteers; however, two of them who took the dose daily for 5 or more days developed headache, lassitude, and malaise after 5 to 7 days. The symptoms corresponded to blood levels of 20 ppm with peaks of 40 and 48 ppm.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ Diets containing 0.25% DNOC (or 2500 mg/kg feed) were administered for 2 days to 5-day-old white Peking ducklings. Cataracts were produced within 24 hr in all the birds. This concentration induced 56% mortality the first day and 100% the second day.

Human Toxicity Values:

Quantitative human toxicity values (e.g., lethal dose) for this compound.

>> The lethal dose in humans is reported to lie in the range of 350 to 3000 mg.

Non-Human Toxicity Values:

>> LD50 Rat oral 10 mg/kg.

12. Ecological Information

Resident Soil (mg/kg)

>> 5.10e+00

Industrial Soil (mg/kg)

>> 6.60e+01

Tapwater (ug/L)

>> 1.50e+00

MCL (ug/L)

>> 5.00e+00

Risk-based SSL (mg/kg)

>> 2.60e-03

Chronic Oral Reference Dose (mg/kg-day)

>> 8e-05

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 very toxic to aquatic organisms.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> 4,6-Dinitro-o-cresol was detected, not quantified in the sediment-soil-water complex at the Love Canal, Buffalo, NY(1).

13. Disposal Considerations

Spillage Disposal

>> Personal protection: chemical protection suit including self-contained breathing apparatus. 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

>> Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number P047, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

>> Product: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Contaminated packaging: Dispose of as unused product.

>> 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.

>> Dinitrocresol is a waste chemical stream constituent which may be subjected to ultimate disposal by controlled incineration. Incinerate (1,000 °F minimum) with adequate scrubbing and ash disposal facilities.

>> A potential candidate for rotary kiln incineration at a temperature range of 820 to 1,600 °C and residence times of seconds for liquids and gases, and hours for solids. A potential candidate for fluidized bed incineration at a temperature range of 450 to 980 °C and residence times of seconds for liquids and gases, and longer for solids.

14. Transport Information

DOT

4,6-Dinitro-o-cresol and salts
6.1
UN Pack Group: II
Reportable Quantity of 10 lb or 4

IATA

4,6-Dinitro-o-cresol and salts
6.1,
UN Pack Group: II

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.

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

Regulatory Information

REACH Registered Substance

>> Status: Active Update: 30-09-2010 https://echa.europa.eu/registration-dossier/-/registered-dossier/10481

New Zealand EPA Inventory of Chemical Status

>> 4,6-Dinitro-o-cresol: HSNO Approval: HSR002979 Approved with controls

16. Other Information

Other Safety Information

Chemical Assessment

>> IMAP assessments - Phenol, 2-methyl-4,6-dinitro-: Human health tier I assessment

>> IMAP assessments - Phenol, 2-methyl-4,6-dinitro-: 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."