

1. Material Identification

Product Name : Cyanazine

Catalog Number : io-2056

CAS Number : 21725-46-2

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

>> H301 (31.1%): Toxic if swallowed [Danger Acute toxicity, oral]

>> H302 (68.9%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H312 (31.1%): Harmful in contact with skin [Warning Acute toxicity, dermal]

>> H332 (31.1%): Harmful if inhaled [Warning Acute toxicity, inhalation]

>> H400 (100%): 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

>> P261, P264, P270, P271, P273, P280, P301+P316, P301+P317, P302+P352, P304+P340, P317, P321, P330, P362+P364, P391, P405, and P501

Health Hazards:

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

>> TOXIC and/or CORROSIVE; inhalation, ingestion or skin contact with material may cause severe injury or death. Contact with molten substance may cause severe burns to skin and eyes. Avoid any skin contact. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause environmental contamination. (ERG, 2024)

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

>> Non-combustible, substance itself does not burn but may decompose upon heating to produce corrosive and/or toxic fumes. Some are oxidizers and may ignite combustibles (wood, paper, oil, clothing, etc.). Corrosives in contact with metals may evolve flammable hydrogen gas. Containers may explode when heated. For electric vehicles or equipment,

ERG Guide 147 (lithium ion or sodium ion batteries) or ERG Guide 138 (sodium batteries) should also be consulted. (ERG, 2024)

>> Not combustible. Liquid formulations containing organic solvents may be flammable.

3. Composition/Information On Ingredients

Chemical name : Cyanazine
CAS Number : 21725-46-2
Molecular Formula : C₉H₁₃CIN₆
Molecular Weight : 240.6900 g/mol

4. First Aid Measures

First Aid:

- >> Excerpt from ERG Guide 154 [Substances – Toxic and/or Corrosive (Non-Combustible)]:
- >> Refer to the "General First Aid" section. Specific First Aid: For corrosives, in case of contact, immediately flush skin or eyes with running water for at least 30 minutes. Additional flushing may be required. (ERG, 2024)

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

- >> Refer for medical attention .

5. Fire Fighting Measures

- >> 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.

- >> Do NOT wash away into sewer. 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:

- >> Provision to contain effluent from fire extinguishing. Separated from food and feedstuffs. Cool. Dry.

Storage Conditions:

- >> Keep from domestic animals, particularly cattle.

8. Exposure Control/ Personal Protection

- >> 0.1 [mg/m³], inhalable particulate matter
- >> 0,1 mg/m

Inhalation Risk:

- >> Evaporation at 20 °C is negligible; a harmful concentration of airborne particles can, however, be reached quickly.

Effects of Long Term Exposure:

- >> Animal tests show that this substance possibly causes malformations in human babies.

Exposure Prevention

- >> AVOID EXPOSURE OF (PREGNANT) WOMEN! IN ALL CASES CONSULT A DOCTOR!

Inhalation Prevention

- >> Use local exhaust or breathing protection.

Skin Prevention

- >> Protective gloves. Protective clothing.

Eye Prevention

- >> Wear safety spectacles.

Ingestion Prevention

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

9. Physical And Chemical Properties

Molecular Weight:

- >> 240.69

Exact Mass:

>> 240.0890221

Physical Description:

- >> Cyanazine appears as colorless crystals. Non corrosive when dry. Used as a selective systemic herbicide.
- >> WHITE CRYSTALLINE POWDER.

Color/Form:

- >> White crystals

Melting Point:

- >> 167.5–169 °C
- >> 168 °C

Solubility:

- >> Solubility at 25 °C (g/l) in: benzene, 15; chloroform, 210; ethanol, 45; hexane, 15.
- >> Solubility in water, g/100ml at 25 °C: 0.02

Density:

- >> 1.29 kg/l @ 20 °C
- >> 1.26 g/cm³

Vapor Pressure:

- >> 0.00000014 [mmHg]
- >> Vapor pressure at 20 °C: negligible

LogP:

- >> log Kow= 2.22
- >> 2.24

Stability/Shelf Life:

- >> Very stable to heat and UV light. Stable between pH 5 and 9, but hydrolyzed by strong acids and alkalis.

Decomposition:

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

Corrosivity:

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

- >> Formulated products are noncorrosive

Dissociation Constants:

- >> pKa = 0.87

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.

- >> 162.93 Å² [M+Na]⁺
- >> 155.79 Å² [M+H]⁺

10. Stability And Reactivity

- >> Stable at pHs between 5.0 and 9.0, but is hydrolyzed by strong acids and bases.

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)

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

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

Chemical

>> Cyanazine

USGS Parameter Code

>> 66592

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

>> 10

Cancer HBSL [µg/L]

>> 0.03-3

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).

Exposure Routes:

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

Adverse Effects:

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

>> Reproductive Toxin – A chemical that is toxic to the reproductive system, including defects in the progeny and injury to male or female reproductive function. Reproductive toxicity includes developmental effects. See Guidelines for Reproductive Toxicity Risk Assessment.

>> ACGIH Carcinogen – Confirmed Animal.

Toxicity Data:

>> LCLo (rat) > 4,900 mg/m³

Antidote and Emergency Treatment:

>> Skin decontamination: Skin contamination should be treated promptly by washing with soap and water. Contamination of the eyes should be treated immediately by prolonged flushing of the eyes with large amounts of clean water. If dermal or ocular irritation persists, medical attention should be obtained without delay.

Non-Human Toxicity Excerpts:

>> In 2 year feeding trials, no effect level for rats was 12 mg/kg diet, and for dogs 25 mg/kg diet.

Non-Human Toxicity Values:

>> LD50 Rat oral 288 mg/kg

12. Ecological Information**Resident Soil (mg/kg)**

>> 6.50e-01

Industrial Soil (mg/kg)

>> 2.70e+00

Tapwater (ug/L)

>> 8.80e-02

MCL (ug/L)

>> 1.30e+03

Risk-based SSL (mg/kg)

>> 4.1e-05

Oral Slope Factor (mg/kg-day)-1

>> 8.40e-01

Chronic Oral Reference Dose (mg/kg-day)

>> 2.00e-03

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Fraction of Contaminant Absorbed Dermal from Soil

>> 0.1

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.

>> SEDIMENT: Cyanazine was not detected in sediment samples collected from a small agricultural catchment in Sweden between 1990-1991 (detection limit 20-100 ug/kg, dry weight); the average concentration of cyanazine in surface water within the catchment was 0.09 to 0.03 ug/l for 1990 and 1991, respectively(1). Cyanazine was found at 90 percent of the sites examined in a survey of 28 agrochemical dealerships in Iowa; the maximum concentration was 4,600 ppb(2).

13. Disposal Considerations**Spillage Disposal**

>> Do NOT wash away into sewer. 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: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with

environmental regulatory agencies for guidance on acceptable disposal practices.

14. Transport Information

DOT

Cyanazine

6.1

UN Pack Group: III

IATA

Cyanazine

6.1,

UN Pack Group: III

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 1 ug/l

Regulatory Information

New Zealand EPA Inventory of Chemical Status

>> Cyanazine: 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 - Propanenitrile, 2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methyl-: Environment tier I assessment
- >> IMAP assessments - Propanenitrile, 2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methyl-: Human health tier I assessment

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