ionz

SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : Adipic Acid
Catalog Number : io-1674
CAS Number : 124-04-9
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)

Note

>> Pictograms displayed are for > 99.9% (5538 of 5540) of reports that indicate hazard statements. This chemical does not meet GHS hazard criteria for < 0.1% (2 of 5540) of reports.

Pictogram(s)

>> Warning

GHS Hazard Statements

>> H319 (95.9%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]

Precautionary Statement Codes

>> P264+P265, P280, P305+P351+P338, and P337+P317

NFPA 704 Diamond

NFPA Health Rating

>> 0 - Materials that, under emergency conditions, would offer no hazard beyond that of ordinary combustible materials.

NFPA Fire Rating

>> 1 - Materials that must be preheated before ignition can occur. Materials require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur.

NFPA Instability Rating

>> 0 - Materials that in themselves are normally stable, even under fire conditions.

EPA Safer Chemical:

EPA labels products so that consumers can easily choose ones that are safer for people and the environment. When consumers see the Safer Choice label on a product, they can be confident that the ingredients have been through a rigorous EPA review. The label means that EPA scientists have evaluated every ingredient in the product to ensure it meets Safer Choice's stringent criteria. When people use Safer Choice products, they are protecting their families and the environment by making safer chemical choices.

EPA Safer Chemical

>> Chemical: Adipic acid

>> Green circle - The chemical has been verified to be of low concern based on experimental and modeled data.

Health Hazards:

>> Inhalation of vapor irritates mucous membranes of the nose and lungs, causing coughing and sneezing. Contact with liquid irritates eyes and has a pronounced drying effect on the skin; may produce dermatitis. (USCG, 1999)

>> Behavior in Fire: Melts and may decompose to give volatile acidic vapors of valeric acid and other substances. Dust may form explosive mixture with air. (USCG, 1999)

>> Combustible. Finely dispersed particles form explosive mixtures in air.

3. Composition/Information On Ingredients

Chemical name : Adipic Acid
CAS Number : 124-04-9
Molecular Formula : C6H10O4
Molecular Weight : 146.1400 g/mol

4. First Aid Measures

First Aid:

>> INHALATION: remove victim to fresh air; get medical attention if irritation persists.

>> EYES: flush with water for at least 15 min.

>> SKIN: flush with water. (USCG, 1999)

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

>> Rinse mouth. Rest. Refer for medical attention .

5. Fire Fighting Measures

>> 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)

>> Use water spray, powder, foam, 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 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.

>> Sweep spilled substance into covered plastic containers. If appropriate, moisten first to prevent dusting. Wash away remainder with plenty of water.

7. Handling And Storage

Storage Conditions:

>> Conditions for safe storage, including any incompatibilities: Keep container tightly closed in a dry and well-ventilated place. Storage class (TRGS 510): Non Combustible Solids.

8. Exposure Control/ Personal Protection

>> 5.0 [mg/m3]

>> 5 mg/m

TLV-TWA (Time Weighted Average)

>> 5 mg/m³ [1990]

Inhalation Risk:

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

Effects of Short Term Exposure:

>> The substance is irritating to the eyes and respiratory tract. Inhalation of the aerosol may cause asthmatic reactions.

Effects of Long Term Exposure:

>> Repeated or prolonged contact may cause skin sensitization. Repeated or prolonged inhalation may cause asthma.

Fire Prevention

>> NO open flames. Closed system, dust explosion-proof electrical equipment and lighting. Prevent deposition of dust. Prevent build-up of electrostatic charges (e.g., by grounding).

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.

Exposure Control and Personal Protection

Maximum Allowable Concentration (MAK)

>> 2.0 [mg/m3], inhalable fraction of the aerosol[German Research Foundation (DFG)]

9. Physical And Chemical Properties

Molecular Weight:

>> 146.14

Exact Mass:

>> 146.05790880

Physical Description:

>> Adipic acid is a white crystalline solid. It is insoluble in water. The primary hazard is the threat to the environment. Immediate steps should be taken to limit its spread to the environment. It is used to make plastics and foams and for other uses.

>> ODOURLESS COLOURLESS CRYSTALLINE POWDER.

Color/Form:

>> Monoclinic prisms from ethyl acetate, water, or acetone and petroleum ether

Odor:

>> Odorless

Taste:

The sensation of flavor perceived in the mouth and throat on contact with a substance.

>> TART TASTE

Boiling Point:

>> 337.5 °C at 760 mm Hg: 265 °C at 100 mm Hg: 240.5 °C at 40 mm Hg: 222 °Cat 20 mm Hg: 205.5 °C at 10 mm Hg; 191 °C at 5 mm Hg; 159.5 °C at 1.0 mm Hg

>> 338 °C

Melting Point:

>> 304 °F (USCG, 1999)

>> 152 °C

Flash Point:

>> 376 °F Combustible solid (USCG, 1999)

>> 196 °C c.c.

Solubility:

>> Slightly soluble in water. Freely soluble in ethanol

>> Solubility in water, g/100ml at 15 °C: 1.4 (moderate)

Density:

>> 1.36 at 68 °F (USCG, 1999) - Denser than water; will sink

>> 1.36 g/cm³

Vapor Density:

>> 5.04 (Air = 1)

>> Relative vapor density (air = 1): 5.04

Vapor Pressure:

>> 3.02X10-5 Pa at 25 °C (2.27X10-7 mm Hg)

>> Vapor pressure, Pa at 18.5 °C: 10

LogP:

>> log Kow = 0.08

>> 0.08

Stability/Shelf Life:

>> Stable under recommended storage conditions.

Autoignition Temperature:

>> 788 °F; 450 °F (USCG, 1999)

>> 422 °C

Decomposition:

>> Melts and may decompose to give volatile acidic vapors of valeric acid and other substances.

Viscosity:

>> Viscosity of melt: 4.54 cP at 160 °C; 2.64 cP at 193 °C

Corrosivity:

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

>> Corrosion rate for ASTM grade 2 Titanium: 0.0 mm/yr at 232 °C for 67% (wt) concn.

Heat of Combustion:

>> -2800 kJ/mol

Heat of Vaporization:

>> 549 kJ/kg

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.

>> pH of saturated aqueous solution at 25 °C = 2.7; pH of 0.1% solution at 25 °C = 3.2

Ionization Efficiency:

The ratio of the number of ions formed to the number of electrons or photons used in an ionization process.

Ionization mode

>> Positive

logIE

>> -0.28

pH

>> 2.7

Instrument

>> Agilent XCT

Ion source

>> Electrospray ionization

Additive

>> formic acid (5.3nM)

Organic modifier

>> MeCN (80%)

Reference

>> DOI:

Dissociation Constants:

>> K1 = 3.90X10-5 at 25 °C; K2 = 5.29X10-6 at 25 °C

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.

>> 129.61 Å² [M+Na-2H]- [CCS Type: DT; Method: single field calibrated with Agilent tune mix (Agilent)]

10. Stability And Reactivity

>> Dust may form explosive mixture with air (USCG, 1999). Insoluble in water.

11. Toxicological Information

Toxicity Summary:

>> IDENTIFICATION AND USE: Adipic acid is white crystalline solid. The major markets for adipic acid include use as feedstocks for nylon 6,6 resins and fibers, polyester polyols and plasticizers. Nylon 6,6 fibers and engineering resins accounted for approximately 85% of total adipic acid consumption in 2011. Polyester polyols and plasticizers, which combined accounted for 24-32% of global adipic acid consumption in 2010 . Other applications documented for adipic acid are as a lubricant additive in coatings, and foams, and in shoe soles, as tanning agent in leather industry, pH regulator in processes such as in the production of cleaning agents, pelletizing agent in disinfectant pills for drinking water, additive in flue gas sulfurization, in the coating of dishwashing machine tablets and as an additive in chemicals. Adipic acid has been identified as being used in hydraulic fracturing as a gelling agent. HUMAN EXPOSURE AND TOXICITY: Adipic acid exhibits an asthma hazard index of 0.75 using the chemical asthma hazard assessment program. Substances with indices of >0.5 have a high probability of being an asthmagen. Threshold for irritation of the human eye was 20 mg/cu m. ANIMAL STUDIES: Adipic acid is slightly toxic on acute exposure but produces moderate to severe eye irritation in rabbits (20 mg/24 hr). High concentrations of adipic acid can cause persistent pulmonary structural and functional alterations. In both mice and rabbits, lethal doses produce signs of inactivity, stomach and intestinal distention, and irritation and hemorrhage of the intestines. A group of mice received intravaginally, three time weekly, applications of a powdered mixture containing urea, adipic acid, and carboxymethyl cellulose. There was a high incidence of vaginal cancer after prolonged treatment. Experiments extended over one year, in which the three ingredients were given separately, yielded no tumors. Adipic acid is not mutagenic in Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, and TA1538 or in Escherichia coli (WP2(uvrA)) with or without rat microsomal activation. ECOTOXICITY STUDIES: Adipic acid is slightly to moderately toxic to fish, daphnia, and algae in acute tests.

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

>> Hexanedioic Acid

Reference Dose (RfD), Chronic

>> 2 mg/kg-day

Reference Dose (RfD), Subchronic

>> 2 mg/kg-day

PPRTV Assessment

>> PDF Document

Last Revision

>> 2006

Exposure Routes:

>> The substance can be absorbed into the body by inhalation of its aerosol.

Inhalation Exposure

>> Cough. Sore throat.

Eye Exposure

>> Redness. Pain.

Adverse Effects:

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

>> Asthma - Reversible bronchoconstriction (narrowing of bronchioles) initiated by the inhalation of irritating or allergenic agents.

Interactions:

>> A group of mice received intravaginally, three time weekly, applications of a powdered mixture containing urea, adipic acid, and carboxymethyl cellulose. There was a high incidence of vaginal cancer after prolonged treatment. Experiments extended over one year, in which the three ingredients were given separately, yielded no tumors.

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 if 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 victim quiet and maintain normal body temperature. Obtain medical attention. /Organic acids and related compounds/

Human Toxicity Excerpts:

>> /CASE REPORTS/ We present the first case of occupational asthma to colophony-free solder wire containing an adipic acid flux, previously only reported in a pharmaceutical factory worker who was in contact with spiramycin powder. The 43-yr-old female presented with rhinitic symptoms in 1992. She had worked as a solderer and desolderer of alternator parts since June 1989. The process used a colophony-free solder wire containing an adipic acid flux from 1996, but, when desoldering, colophony fluxes may still have been present. From 1998, she experienced a gradual onset of breathlessness and chest tightness, which she noticed was affecting her keep-fit. She had had no asthma, hay fever or eczema in childhood, and there was no family history of these conditions. She was a lifelong nonsmoker and gave negative skin-prick test results to common environmental allergens. She started to show nocturnal waking and shortness of breath in the morning, feeling better on days away from work, particularly on holiday. She also noticed that she felt better when not soldering at work. She carried out serial peak expiratory flow measurements four times daily for a total of 4 weeks. When plotted using the Oasys program, they showed work-related changes, with an Oasys score of 3.1 (probable occupational asthma; a score of >2.50 has a sensitivity of 75% and specificity of 94% for occupational asthma diagnosis) and an area between the curves (ABC) score of 15 L/min x hr (an ABC score of >/= 15 L/min x hr has a sensitivity of 69% and specificity of 100%). She was admitted for specific inhalation challenge testing to colophony- and adipic-acid-fluxed solder wires. She melted /about/ 1 m of solder wire (using an iron heated to 170 °C) over three challenges, totalling 30 min for the colophony-containing wire and 12 min for the adipic acid wire. ... She exhibited a late asthmatic reaction after the adipic acid exposure, with her forced expiratory volume in 1 sec falling by a maximum of 28% from baseline. She showed no reaction to the colophony-fluxed solder wire. Her methacholine reactivity before challenge was 3,450 ug methacholine (normal) using the method of Yan et al., halving following adipic acid wire challenge to 1,729 ug (mildly hyperreactive). Adipic acid exhibits an asthma hazard index of 0.75 using the chemical asthma hazard assessment program. Substances with indices of >0.5 have a high probability of being an asthmagen. Other non-colophony-based fluxes, such as palmitic acid and dodecanedioic acid, also have high hazard indices (0.92 and 0.94, respectively). On follow-up, the worker had joined a different company as a toilet cistern assembler. She still showed significant asthma, with occasional nocturnal wakening and a St George's Respiratory Questionnaire score of 50.8. Her methacholine reactivity was normal at >4,800 ug. Thus adipic-acid-fluxed solder wire is a new cause of occupational asthma.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ Single intratracheal instillation of either 2.5, 5, or 7 mg of adipic acid in rats produced acute pulmonary cytotoxicity and inflammation. One day after instillation, lavage protein, LDH, and inflammatory cells were markedly increased. Histopathology confirmed acute pulmonary inflammation. Four weeks after exposure, pulmonary alterations persisted and were most pronounced in the rats receiving 7 mg. Significant changes

included hydroxyproline increases, histologic foci of pulmonary fibrosis, and persistent tachypnea. Neutralization of the pH ameliorated the toxicity. These findings suggest that high concentrations of adipic acid can cause persistent pulmonary structural and functional alterations. This is most likely the result of the acidity and lipid solubility of this organic acid.

Non-Human Toxicity Values:

>> Rat: inhalation: no effect level: 126 g/L, 15 x 6 hr (as in source)

12. Ecological Information

Resident Soil (mg/kg)

>> 1.30e+05

Industrial Soil (mg/kg)

>> 1.60e+06

Tapwater (ug/L)

>> 4.00e+04

MCL (ug/L)

>> 5.00e+01

Risk-based SSL (mg/kg)

>> 9.90e+00

Chronic Oral Reference Dose (mg/kg-day)

>> 2.00e+00

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Fraction of Contaminant Absorbed Dermally from Soil

>> 0.1

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> Soil samples taken at the University of California, Los Angeles campus contained 215 and 568 ppb of adipic acid whereas bog sediment samples from the Sierra Nevada foothills contained 2050 ppb(1).

Average Daily Intake:

The average amount of the compound taken into the body through eating, drinking, or breathing.

>> AIR INTAKE: (assume air concn of 0.1 ug/cu m): 2 ug(1); WATER INTAKE: insufficient data; FOOD INTAKE: insufficient data.

13. Disposal Considerations

Spillage Disposal

>> Sweep spilled substance into covered plastic containers. If appropriate, moisten first to prevent dusting. Wash away remainder with plenty of water.

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.

>> 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.

>> Adipic acid is a waste chemical stream constituent which may be subjected to ultimate disposal by controlled incineration.

>> For more Disposal Methods (Complete) data for ADIPIC ACID (6 total), please visit the HSDB record page.

14. Transport Information

DOT

Adipic Acid

Reportable Quantity of 5000 lb or 2270 kg

IATA

Adipic Acid

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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.

>> Adipic 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

The Australian Inventory of Industrial Chemicals

>> Chemical: Hexanedioic acid

REACH Registered Substance

>> Status: Active Update: 18-05-2023 https://echa.europa.eu/registration-dossier/-/registered-dossier/15464

REACH Registered Substance

>> Status: Active Update: 07-12-2010 https://echa.europa.eu/registration-dossier/-/registered-dossier/15698

New Zealand EPA Inventory of Chemical Status

>> Hexanedioic acid: Does not have an individual approval but may be used under an appropriate group standard

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

Other Safety Information

Chemical Assessment

>> IMAP assessments - Hexanedioic acid: Human health tier II assessment

>> IMAP assessments - Hexanedioic acid: 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."