SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : Benzoic acid
Catalog Number : io-1805
CAS Number : 65-85-0
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)

Note

>> Pictograms displayed are for 99.1% (3220 of 3248) of reports that indicate hazard statements. This chemical does not meet GHS hazard criteria for 0.9% (28 of 3248) of reports.

Pictogram(s)

GHS Hazard Statements

>> H302 (30%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H315 (82.7%): Causes skin irritation [Warning Skin corrosion/irritation]

>> H318 (81.2%): Causes serious eye damage [Danger Serious eye damage/eye irritation]

>> H319 (16.5%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]

>> H372 (19.9%): Causes damage to organs through prolonged or repeated exposure [Danger Specific target organ toxicity, repeated exposure]

Precautionary Statement Codes

>> P260, P264, P264+P265, P270, P280, P301+P317, P302+P352, P305+P351+P338, P305+P354+P338, P317, P319, P321, P330, P332+P317, P337+P317, P362+P364, and P501

NFPA 704 Diamond

NFPA Health Rating

>> 1 - Materials that, under emergency conditions, can cause significant irritation.

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: Benzoic acid

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

Health Hazards:

>> Dust may be irritating to nose and eyes. At elevated temperatures, fumes may cause irritation of eyes, respiratory system, and skin. (USCG, 1999)

>> Behavior in Fire: Vapor from molten benzoic acid may form explosive mixture with air. Concentrated dust may form explosive mixture. (USCG, 1999)

>> Combustible. Finely dispersed particles form explosive mixtures in air. Risk of fire and explosion on contact with incompatible substances. See Chemical Dangers.

3. Composition/Information On Ingredients

Chemical name : Benzoic acid
CAS Number : 65-85-0
Molecular Formula : C7H6O2
Molecular Weight : 122.1200 g/mol

4. First Aid Measures

First Aid:

>> EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.

>> SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment.

>> INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing.

>> INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital. (NTP, 1992)

First Aid Measures

Inhalation First Aid

>> Fresh air, rest.

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

>> Use water spray, powder, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

6. Accidental Release Measures

Spillage Disposal:

Methods for containment and safety measures to protect workers dealing with a spillage of this chemical.

>> Personal protection: protective clothing and face shield. Do NOT let this chemical enter the environment. Sweep spilled substance into covered plastic containers. Carefully collect remainder in covered containers. If appropriate, moisten first to prevent dusting. Then store and dispose of according to local regulations.

7. Handling And Storage

Safe Storage:

>> Store only in original container. Separated from incompatible materials. See Chemical Dangers. Fireproof. Store in an area without drain or sewer access.

Storage Conditions:

>> The bulk material should be stored in well-closed container in a cool dry place.

8. Exposure Control/ Personal Protection

>> 0.5 [mg/m3], inhalable fraction and vapor

>> 0.5 mg/m

MAK (Maximale Arbeitsplatz Konzentration)

>> (respirable fraction): 0.5 mg/m

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.

Effects of Short Term Exposure:

>> The substance is severely irritating to the eyes. The substance is mildly irritating to the skin. Exposure could cause a non-allergic rash on contact.

Effects of Long Term Exposure:

>> Lungs may be affected by repeated or prolongated exposure to an aerosol of this substance.

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.

>> EPA RfD= 4.0 mg/kg

Fire Prevention

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

Exposure Prevention

>> PREVENT DISPERSION OF DUST! STRICT HYGIENE!

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.

Exposure Control and Personal Protection

Maximum Allowable Concentration (MAK)

>> 0.5 [mg/m3], respirable fraction (2 mg/m3, inhalable fraction)[German Research Foundation (DFG)]

9. Physical And Chemical Properties

Molecular Weight:

>> 122.12

Exact Mass:

>> 122.036779430

Physical Description:

>> Benzoic acid appears as a white crystalline solid. Slightly soluble in water. The primary hazard is the potential for environmental damage if released. Immediate steps should be taken to limit spread to the environment. Used to make other chemicals, as a food preservative, and for other uses.

>> WHITE CRYSTALS OR POWDER.

Color/Form:

>> Monoclinic tablets, plates, leaflets

Odor:

>> Odorless or with a slight benzaldehyde odor

Taste:

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

>> ALMOST TASTELESS /BENZOIC ACID USP/

Boiling Point:

>> 480 °F at 760 mmHg (NTP, 1992)

>> 249 °C

Melting Point:

>> 252.3 °F (NTP, 1992)

>> 122 °C

Flash Point:

>> 250 °F (NTP, 1992)

>> 121 °C c.c.

Solubility:

>> less than 1 mg/mL at 68 °F (NTP, 1992)

>> Solubility in water, g/l at 20 °C: 3 (slightly soluble)

Density:

>> 1.316 at 82.4 °F (USCG, 1999) - Denser than water; will sink

>> 1.3 g/cm^3

Vapor Density:

>> 4.21 (NTP, 1992) - Heavier than air; will sink (Relative to Air)

>> Relative vapor density (air = 1): 4.2

Vapor Pressure:

>> 1 mmHg at 205 °F (NTP, 1992)

>> Vapor pressure, Pa at 25 °C: 0.1

LogP:

>> 1.87

LogS:

The base-10 logarithm of the aqueous solubility of this compound.

Stability/Shelf Life:

>> A 0.1% w/v aqueous solution of benzoic acid has been reported to be stable for at least 8 weeks when stored in polyvinyl chloride bottels, at room temperature.

Autoignition Temperature:

>> 1063 °F (USCG, 1999)

>> 570 °C

Decomposition:

>> When heated to decomp it emits acrid smoke and irritating fumes.

Viscosity:

>> 1.26 cP at 130 °C

Heat of Combustion:

>> 3227 kJ/mole

Heat of Vaporization:

>> 534 KJ/mol at 140 °C, 425 Kj/mol at 249 °C

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.

>> About 4 (solution in water)

Surface Tension:

>> 31 mN/m at 130 °C

Ionization Efficiency:

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

Ionization mode

>> Negative

logIE

>> 0.0

pH

>> 10.5

Instrument

>> Agilent XCT

Ion source

>> Electrospray ionization

Additive

>> ammonia (10nM)

Organic modifier

>> MeCN (80%)

Reference

>> DOI:10.1021/acs.analchem.7b00595

Refractive Index:

>> Index of refraction = 1.504 at 132 °C/D

Dissociation Constants:

Acidic pKa

>> 4.207

pKa

>> 4.19 (at 25 °C)

>> pKa = 4.204 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.

>> 122.35 Å² [M+H]+ [CCS Type: TW; Method: calibrated with polyalanine and drug standards]

>> 122.33 Å² [M+H]+ [CCS Type: TW; Method: calibrated with polyalanine and drug standards]

>> 121.74 Å² [M+H]+ [CCS Type: TW; Method: calibrated with polyalanine and drug standards]

>> 124.27 Å² [M+H]+ [CCS Type: TW; Method: calibrated with polyalanine and drug standards]

>> 124.3 Å² [M+H]+ [CCS Type: TW; Method: calibrated with polyalanine and drug standards]

10. Stability And Reactivity

>> Vapor from molten benzoic acid may form explosive mixture with air. The finely powdered dry acid is a significant dust explosion hazard [Bretherick, 5th ed., 1995, p. 884]. In air very rapid combustion occurs [Wilson, L.Y. et al., J. Chem. Ed., 1985, 62(10), p. 902]. Slightly soluble in water.

11. Toxicological Information

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

>> Benzoic Acid

Reference Dose (RfD), Subchronic

>> 4 mg/kg-day

Reference Concentration (RfC), Subchronic

>> 2 x 10^-3 mg/m^3

PPRTV Assessment

>> PDF Document

Last Revision

>> 2005

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).

Exposure Routes:

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

Inhalation Exposure

>> Sore throat. Cough.

Skin Exposure

>> Redness. Swelling. Itching.

Eye Exposure

>> Redness. Pain. Corneal damage.

Ingestion Exposure

>> Abdominal pain. Nausea. Vomiting.

Adverse Effects:

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

>> ACGIH Carcinogen - Not Suspected.

Toxicity Data:

>> LC50 (rat) = >26 mg/m3/1H

Interactions:

>> The metabolism of the benzoates depletes glycine concentrations and can therefore alter the glycine-dependent metabolism of other compounds. /Investigators/ demonstrated that benzoic acid or sodium benzoate successfully competed with aspirin for glycine, resulting in increased concentration and persistence of salicylic acid in the body. Almost total inhibition of salicyluric acid formation in humans was achieved using either 2.7 g benzoic acid or 3.2 g sodium benzoate.

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. /Organic acids and related compounds/

Human Toxicity Excerpts:

>> /HUMAN EXPOSURE STUDIES/ In nine patients on penicillin treatment given 12,000 mg benzoic acid divided into eight doses over 5 days in eight subjects and over 14 days in one subject, no adverse effects on blood urea nitrogen or

creatinine clearance were reported.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ In a limit test with rabbits, no mortality or signs of intoxication were seen after dermal application of 10,000 mg/kg bodyweight. The gross autopsy gave no significant findings.

Non-Human Toxicity Values:

>> LD50 Cat oral 2000 mg/kg

TSCA Test Submissions:

Under the Toxic Substances Control Act (TSCA), EPA has broad authority to issue regulations designed to require manufacturers (including importers) or processors to test chemical substances and mixtures for health and environmental effects. This section provides information on test reports submitted for this chemical under TSCA.

>> The effects of subchronic exposure to benzoic acid (BA) were evaluated in male and female Sprague-Dawley rats (10/sex/group) exposed by inhalation to 0, 0.025, 0.25 or 1.2 mg BA/L (generated as a dust aerosol with an equivalent aerodynamic diameter of 4.7 um) for 6 hrs/day, 5 days/week for 4 weeks. All high- and mid-dose animals exhibited upper respiratory tract irritation (red material around the nares). Two animals (1/sex) died in the high-dose group. There were statistically significant differences observed between treated and control animals in the following (high-dose group unless noted otherwise): decreased body weight gain, random differences in hematological data and serum biochemical evaluation (not considered to be exposure related except for a related decrease in the number of platelets), and decreased absolute and relative weights of liver (males), kidney (females, high- and mid-dose levels), and trachea/lung (females). The incidence of slight multifocal and generalized interstitial fibrosis and inflammatory cell infiltrate in treated animals were high compared to controls (not dose-related). No compound-related macroscopic lesions were observed in any of the rats. There were no deaths, no significant effects on body weight gain, and there were no significant effects on hematologic or biochemical parameters in the low- or mid-dose animals relative to the negative controls.

12. Ecological Information

Resident Soil (mg/kg)

>> 2.50e+05

Industrial Soil (mg/kg)

>> 3.30e+06

Tapwater (ug/L)

>> 7.50e+04

MCL (ug/L)

>> 5.00e+00

Risk-based SSL (mg/kg)

>> 1.50e+01

Chronic Oral Reference Dose (mg/kg-day)

>> 4.00e+00

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.

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

>> Benzoic acid has been detected but not quantified in mollusks and crustaceans(1).

Average Daily Intake:

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

>> The average daily intake of benzoic acid is 312 mg of which 278 mg is absorbed as sodium benzoate and 34 mg as benzoic acid(1).

13. Disposal Considerations

Spillage Disposal

>> Personal protection: protective clothing and face shield. Do NOT let this chemical enter the environment. Sweep spilled substance into covered plastic containers. Carefully collect remainder in covered containers. If appropriate, moisten first to prevent dusting. Then store and dispose of according to local regulations.

Disposal Methods

>> 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.

>> The following wastewater treatment technologies have been investigated for benzoic acid: concentration process: biological treatment.

>> Incineration: Waste material can be burned in an approved incinerator with an afterburner, as a soln in a flammable solvent or as a solid packaged in paper, plastic or cardboard.

>> The following wastewater treatment technologies have been investigated for benzoic acid: concentration process: activated carbon.

>> The following wastewater treatment technologies have been investigated for benzoic acid: concentration process: resin adsorption.

14. Transport Information

DOT

Benzoic acid

Reportable Quantity of 5000 lb or 2270 kg

IATA

Benzoic 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.

>> Benzoic 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: Benzoic acid

REACH Registered Substance

>> Status: Active Update: 30-10-2022 https://echa.europa.eu/registration-dossier/-/registered-dossier/13124

New Zealand EPA Inventory of Chemical Status

>> Benzoic acid: 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 - Benzoic acid: Environment tier I assessment

>> IMAP assessments - Benzoic acid: Human health tier II 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."