SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : iso-Butyric acid
Catalog Number : io-1893
CAS Number : 79-31-2
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

>> H226 (11.1%): Flammable liquid and vapor [Warning Flammable liquids]

>> H302 (99.2%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H311 (10.5%): Toxic in contact with skin [Danger Acute toxicity, dermal]

>> H312 (89.5%): Harmful in contact with skin [Warning Acute toxicity, dermal]

Precautionary Statement Codes

>> P210, P233, P240, P241, P242, P243, P262, P264, P270, P280, P301+P317, P302+P352, P303+P361+P353, P316, P317, P321, P330, P361+P364, P362+P364, P370+P378, P403+P235, P405, and P501

NFPA 704 Diamond

NFPA Health Rating

>> 3 - Materials that, under emergency conditions, can cause serious or permanent injury.

NFPA Fire Rating

>> 2 - Materials that must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur. Materials would not under normal conditions form hazardous atmospheres with air, but under high ambient temperatures or under moderate heating could release vapor in sufficient quantities to produce hazardous atmospheres with air.

NFPA Instability Rating

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

Health Hazards:

>> Inhalation causes irritation of nose and throat. Ingestion causes irritation of mouth and stomach. Contact with eyes or skin causes irritation. (USCG, 1999)

ERG 2024, Guide 132 (Isobutyric acid)

>> May cause toxic effects if inhaled or ingested.

>> Contact with substance may cause severe burns to skin and eyes.

>> Fire will produce irritating, corrosive and/or toxic gases.

>> Vapors may cause dizziness or asphyxiation, especially when in closed or confined areas.

>> Runoff from fire control or dilution water may cause environmental contamination.

>> Excerpt from ERG Guide 132 [Flammable Liquids - Corrosive]:

>> Flammable/combustible material. May be ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along the ground and collect in low or confined areas (sewers, basements, tanks, etc.). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids will float on water. (ERG, 2024)

ERG 2024, Guide 132 (Isobutyric acid)

>> Flammable/combustible material.

>> May be ignited by heat, sparks or flames.

>> Vapors may form explosive mixtures with air.

>> Vapors may travel to source of ignition and flash back.

>> Most vapors are heavier than air. They will spread along the ground and collect in low or confined areas (sewers, basements, tanks, etc.).

>> Vapor explosion hazard indoors, outdoors or in sewers.

>> Those substances designated with a (P) may polymerize explosively when heated or involved in a fire.

>> Runoff to sewer may create fire or explosion hazard.

>> Containers may explode when heated.

>> Many liquids will float on water.

>> Flammable. Gives off irritating or toxic fumes (or gases) in a fire. Above 56 °C explosive vapour/air mixtures may be formed.

3. Composition/Information On Ingredients

Chemical name : iso-Butyric acid
CAS Number : 79-31-2
Molecular Formula : C4H8O2
Molecular Weight : 88.1100 g/mol

4. First Aid Measures

First Aid:

>> INHALATION: move to fresh air.

>> INGESTION: give large amounts of water.

>> EYES: flush with water for at least 15 min.; get medical attention if irritation persists.

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

ERG 2024, Guide 132 (Isobutyric acid)

>> General First Aid:

>> Call 911 or emergency medical service.

>> Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and avoid contamination.

>> Move victim to fresh air if it can be done safely.

>> Administer oxygen if breathing is difficult.

>> If victim is not breathing:

>> DO NOT perform mouth-to-mouth resuscitation; the victim may have ingestedor inhaled the substance.

>> If equipped and pulse detected, wash face and mouth, then give artificial respiration using a proper respiratory medical device (bag-valve mask, pocket mask equipped with a one-way valve or other device).

>> If no pulse detected or no respiratory medical device available, provide continuouscompressions. Conduct a pulse check every two minutes or monitor for any signs of spontaneous respirations.

>> Remove and isolate contaminated clothing and shoes.

>> For minor skin contact, avoid spreading material on unaffected skin.

>> In case of contact with substance, remove immediately by flushing skin or eyes with running water for at least 20 minutes.

>> For severe burns, immediate medical attention is required.

>> Effects of exposure (inhalation, ingestion, or skin contact) to substance may be delayed.

>> Keep victim calm and warm.

>> Keep victim under observation.

>> For further assistance, contact your local Poison Control Center.

>> Note: Basic Life Support (BLS) and Advanced Life Support (ALS) should be done by trained professionals.

>> 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.

>> In case of burns, immediately cool affected skin for as long as possible with cold water. Do not remove clothing if adhering to skin.

>> In Canada, an Emergency Response Assistance Plan (ERAP) may be required for this product. Please consult the shipping paper and/or the "ERAP" section.

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

>> Give one or two glasses of water to drink. Do NOT induce vomiting. Refer for medical attention .

5. Fire Fighting Measures

>> Excerpt from ERG Guide 132 [Flammable Liquids - Corrosive]:

>> Some of these materials may react violently with water.

>> SMALL FIRE: Dry chemical, CO2, water spray or alcohol-resistant foam.

>> LARGE FIRE: Water spray, fog or alcohol-resistant foam. If it can be done safely, move undamaged containers away from the area around the fire. Dike runoff from fire control for later disposal. Do not get water inside containers.

>> FIRE INVOLVING TANKS, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. 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. For massive fire, use unmanned master stream devices or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2024)

>> Use alcohol-resistant foam, 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 132 [Flammable Liquids - Corrosive]:

>> IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area for at least 50 meters (150 feet) in all directions.

>> 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)

Evacuation: ERG 2024, Guide 132 (Isobutyric acid)

>> Immediate precautionary measure

>> Isolate spill or leak area for at least 50 meters (150 feet) in all directions.

>> Spill

>> For non-highlighted materials: 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.

Spillage Disposal:

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

>> Remove all ignition sources. Collect leaking and spilled liquid in covered containers as far as possible. Wash away remainder with plenty of water.

Accidental Release Measures

Public Safety: ERG 2024, Guide 132 (Isobutyric acid)

>> CALL 911. Then call emergency response telephone number on shipping paper. If shipping paper not available or no answer, refer to appropriate telephone number listed on the inside back cover.

>> Keep unauthorized personnel away.

>> Stay upwind, uphill and/or upstream.

>> Ventilate closed spaces before entering, but only if properly trained and equipped.

Spill or Leak: ERG 2024, Guide 132 (Isobutyric acid)

>> ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area.

>> All equipment used when handling the product must be grounded.

>> Do not touch or walk through spilled material.

>> Stop leak if you can do it without risk.

>> Prevent entry into waterways, sewers, basements or confined areas.

>> A vapor-suppressing foam may be used to reduce vapors.

>> Absorb with earth, sand or other non-combustible material.

>> For hydrazine, absorb with DRY sand or inert absorbent (vermiculite or absorbent pads).

>> Use clean, non-sparking tools to collect absorbed material.

>> Large Spill

>> Dike far ahead of liquid spill for later disposal.

>> Water spray may reduce vapor, but may not prevent ignition in closed spaces.

7. Handling And Storage

Safe Storage:

>> Fireproof. Separated from strong bases and food and feedstuffs.

8. Exposure Control/ Personal Protection

Emergency Response: ERG 2024, Guide 132 (Isobutyric acid)

>> Some of these materials may react violently with water.

>> Small Fire

>> Dry chemical, CO2, water spray or alcohol-resistant foam.

>> Large Fire

>> Water spray, fog or alcohol-resistant foam.

>> If it can be done safely, move undamaged containers away from the area around the fire.

>> Dike runoff from fire control for later disposal.

>> Do not get water inside containers.

>> Fire Involving Tanks, Rail Tank Cars or Highway Tanks

>> Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles.

>> 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.

>> For massive fire, use unmanned master stream devices or monitor nozzles; if this is impossible, withdraw from area and let fire burn.

Inhalation Risk:

>> No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20 °C.

Effects of Short Term Exposure:

>> The substance is corrosive to the eyes, skin and respiratory tract. Corrosive on ingestion.

Fire Prevention

>> NO open flames, NO sparks and NO smoking. Above 56 °C use a closed system, ventilation and explosion-proof electrical equipment.

Exposure Prevention

>> AVOID ALL CONTACT! IN ALL CASES CONSULT A DOCTOR!

Inhalation Prevention

>> Use ventilation, local exhaust or breathing protection.

Skin Prevention

>> Protective gloves. Protective clothing.

Eye Prevention

>> Wear face shield.

Ingestion Prevention

>> Do not eat, drink, or smoke during work.

Exposure Control and Personal Protection

Protective Clothing: ERG 2024, Guide 132 (Isobutyric acid)

>> Wear positive pressure self-contained breathing apparatus (SCBA).

>> Wear chemical protective clothing that is specifically recommended by the manufacturer when there is NO RISK OF FIRE.

>> Structural firefighters' protective clothing provides thermal protection but only limited chemical protection.

9. Physical And Chemical Properties

Molecular Weight:

>> 88.11

Exact Mass:

>> 88.052429494

Physical Description:

>> Isobutyric acid appears as a colorless liquid with a light odor of rancid butter. Corrosive to metals and tissue.

>> COLOURLESS LIQUID WITH CHARACTERISTIC ODOUR.

Color/Form:

>> Colorless liquid

Odor:

>> Pungent odor like that of butyric acid, but not as unpleasant

Taste:

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

>> CHEESY TASTE

Boiling Point:

>> 309 °F at 760 mmHg (USCG, 1999)

>> 152-155 °C

Melting Point:

>> -51 °F (USCG, 1999)

>> -47 °C

Flash Point:

>> 132 °F (NFPA, 2010)

>> 56 °C c.c.

Solubility:

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

Density:

>> 0.949 at 68 °F (USCG, 1999) - Less dense than water; will float

>> Relative density (water = 1): 0.95

Vapor Density:

>> 3.0

>> Relative vapor density (air = 1): 3.0

Vapor Pressure:

>> 1.81 [mmHg]

>> Vapor pressure, kPa at 14.7 °C: 0.13

LogP:

>> 0.88

LogS:

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

Stability/Shelf Life:

>> Stable during transport.

Autoignition Temperature:

>> 935 °F (USCG, 1999)

>> 481 °C

Decomposition:

>> When heated to decomposition it emits acrid smoke and fumes.

Viscosity:

>> 1.126 mPa.s

Corrosivity:

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

>> /2-Methylpropanoic acid/ is corrosive to metals.

Heat of Vaporization:

>> 11,182.8 g cal/g mole

Surface Tension:

>> 24.4mN/m at 25 °C /Methyl propanoate/

Odor Threshold:

>> Odor Threshold Low: 8.0 [mmHg]

>> [Merck Index] Odor threshold from CHEMINFO

Refractive Index:

>> Index of refraction: 1.3930 at 20 °C/D

Dissociation Constants:

pKa

>> 4.84 (at 20 °C)

>> pKa = 4.84

10. Stability And Reactivity

>> Flammable. Water soluble

11. Toxicological Information

Exposure Routes:

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

Inhalation Exposure

>> Burning sensation. Cough. Sore throat.

Skin Exposure

>> Redness. Skin burns. Pain.

Eye Exposure

>> Pain. Redness. Severe deep burns.

Ingestion Exposure

>> Abdominal pain. Burning sensation. Shock or collapse.

Adverse Effects:

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

>> Dermatotoxin - Skin burns.

>> Toxic Pneumonitis - Inflammation of the lungs induced by inhalation of metal fumes or toxic gases and vapors.

Antidote and Emergency Treatment:

>> /SRP:/ 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/

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ In an open rabbit skin irritation test, isobutyric acid (0.01 mL, 10 mg) caused some necrosis in 24 hr.

Non-Human Toxicity Values:

>> LD50 Rat oral 2518 mg/kg

12. Ecological Information

ICSC Environmental Data:

>> The substance is harmful to aquatic organisms.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> Isobutyric acid was not detected in soil samples from the UCLA campus, Los Angeles, CA tested in October 1984(1).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

>> Isobutyric acid was identified in rotten mussels (Mytilus edulis) at 10.9 ug/g wet weight(1).

Average Daily Intake:

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

>> Annual consumption is 2650.00 lb. Individual consumption is 0.002245 mg/kg/day.

13. Disposal Considerations

Spillage Disposal

>> Remove all ignition sources. Collect leaking and spilled liquid in covered containers as far as possible. Wash away remainder with plenty of water.

Disposal Methods

>> SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. 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 soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

14. Transport Information

DOT

iso-Butyric acid
3
UN Pack Group: III
Reportable Quantity of 5000 lb or 2270 kg

IATA

iso-Butyric acid
3, 8
UN Pack Group: III

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.

>> iso-Butyric 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: Propanoic acid, 2-methyl-

REACH Registered Substance

>> Status: Active Update: 18-10-2021 https://echa.europa.eu/registration-dossier/-/registered-dossier/14591

New Zealand EPA Inventory of Chemical Status

>> Propanoic acid, 2-methyl-: HSNO Approval: HSR001174 Approved with controls

16. Other Information

Toxic Combustion Products:

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

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