

SAFETY DATA SHEET

Version 8.3
Revision Date 09/06/2024
Print Date 11/23/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Isobutyric acid
Product Number : 96499
Brand : Sigma-Aldrich
Index-No. : 607-063-00-9
CAS-No. : 79-31-2

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES
Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 3), H226
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Dermal (Category 3), H311
Skin corrosion (Category 1B), H314

Sigma-Aldrich - 96499

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Serious eye damage (Category 1), H318
Short-term (acute) aquatic hazard (Category 3), H402

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H226	Flammable liquid and vapor.
H302	Harmful if swallowed.
H311	Toxic in contact with skin.
H314	Causes severe skin burns and eye damage.
H402	Harmful to aquatic life.

Precautionary Statements

P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients**3.1 Substances**

Formula : C4H8O2
Molecular weight : 88.11 g/mol
CAS-No. : 79-31-2
EC-No. : 201-195-7
Index-No. : 607-063-00-9

Component	Classification	Concentration
2-methylpropionic acid; isobutyric acid		
	Flam. Liq. 3; Acute Tox. 4; Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Aquatic Acute 3; H226, H302, H311, H314, H318, H402	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures**4.1 Description of first-aid measures****General advice**

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) Foam Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g.

Chemisorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability Recommended storage temperature

-20 °C

Stench. Store under inert gas.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please

contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Chloroprene

Minimum layer thickness: 0.65 mm

Break through time: 30 min

Material tested:KCL 720 Camapren®

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: clear, liquid Color: colorless
b) Odor	stinging
c) Odor Threshold	8.1 ppm
d) pH	2.3 at 500 g/l at 25 °C (77 °F) - DIN 19268
e) Melting point/freezing point	Melting point/ range: -47 °C (-53 °F)
f) Initial boiling point and boiling range	153 - 154 °C 307 - 309 °F at 1,013.25 hPa
g) Flash point	55 °C (131 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 10 %(V) Lower explosion limit: 2 %(V)
k) Vapor pressure	ca.2 hPa at 20 °C (68 °F)
l) Vapor density	3.04 - (Air = 1.0)

m) Density	0.950 g/cm ³ at 20 °C (68 °F) - DIN 51757
Relative density	No data available
n) Water solubility	618 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - completely soluble
o) Partition coefficient: n-octanol/water	log Pow: 1.1 at 25 °C (77 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	455 °C (851 °F) at 1,018 hPa - DIN 51794
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

Surface tension	70.2 mN/m at 1g/l at 20 °C (68 °F) - OECD Test Guideline 115
Dissociation constant	5 at 20.7 °C (69.3 °F) - OECD Test Guideline 112
Relative vapor density	3.04 - (Air = 1.0)

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Isocyanates
bases
Amines
Nitriles
Oxidizing agents
Reducing agents
Metals

10.4 Conditions to avoid

Heat, flames and sparks.
Heating.

10.5 Incompatible materials

Aluminum, Zinc, Metals, (generation of hydrogen)

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 2,230 mg/kg
(OECD Test Guideline 401)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Inhalation: No data available

LD50 Dermal - Rabbit - male - 474 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive - 1 h

(OECD Test Guideline 404)

Remarks: Tendency of poor wound-healing after penetration of the substance.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Corrosive - 8 Days

(Draize Test)

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is

identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

RTECS: NQ4375000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

- Nausea
- Vomiting
- Headache
- Drowsiness
- Unconsciousness

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	static test LC50 - Leuciscus idus (Golden orfe) - 146.6 mg/l - 96 h (DIN 38412 part 15)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 51.25 mg/l - 48 h (DIN 38412)
Toxicity to algae	static test EbC50 - Desmodesmus subspicatus (green algae) - 45.1 mg/l - 72 h (DIN 38412)
Toxicity to bacteria	EC50 - Pseudomonas putida - 57 mg/l - 17 h Remarks: (IUCLID)

12.2 Persistence and degradability

Biodegradability	Result: 100 % - Readily biodegradable. (OECD Test Guideline 301E)
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12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)

UN number: 2529 Class: 3 (8) Packing group: III
Proper shipping name: Isobutyric acid
Reportable Quantity (RQ): 5000 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 2529 Class: 3 (8) Packing group: III EMS-No: F-E, S-C
Proper shipping name: ISOBUTYRIC ACID

IATA

UN number: 2529 Class: 3 (8) Packing group: III
Proper shipping name: Isobutyric acid

SECTION 15: Regulatory information

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
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2-methylpropionic acid; isobutyric acid	79-31-2	5000	5000
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SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Fire Hazard
Acute Health Hazard

SARA 313 : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

US State Regulations

Massachusetts Right To Know

2-methylpropionic acid; isobutyric acid 79-31-2

Massachusetts Right To Know

2-methylpropionic acid; isobutyric acid 79-31-2

Pennsylvania Right To Know

2-methylpropionic acid; isobutyric acid 79-31-2

Pennsylvania Right To Know

2-methylpropionic acid; isobutyric acid 79-31-2

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

New Jersey Right To Know

2-methylpropionic acid; isobutyric acid 79-31-2

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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