

SAFETY DATA SHEET

Version 8.6
Revision Date 03/08/2024
Print Date 07/13/2024

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

1.1 Product identifiers

Product name : Isobutyronitrile

Product Number : I15602
Brand : Aldrich
CAS-No. : 78-82-0

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

Identified uses : Laboratory chemicals, Synthesis of substances

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 2), H225
Acute toxicity, Oral (Category 2), H300
Acute toxicity, Inhalation (Category 2), H330
Acute toxicity, Dermal (Category 2), H310
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

H225

Highly flammable liquid and vapor.

H300 + H310 + H330

Fatal if swallowed, in contact with skin or if inhaled.

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.

P260

Do not breathe mist or vapors.

P262

Do not get in eyes, on skin, or on clothing.

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P271

Use only outdoors or in a well-ventilated area.

P273

Avoid release to the environment.

P280

Wear protective gloves/ eye protection/ face protection.

P284

Wear respiratory protection.

P301 + P310 + P330

IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.

P302 + P350 + P310

IF ON SKIN: Gently wash with plenty of soap and water. Immediately call a POISON CENTER or doctor/ physician.

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.

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 + P233

Store in a well-ventilated place. Keep container tightly closed.

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

Synonyms

: 2-Methylpropionitrile
2-Methylpropanenitrile
Isopropyl cyanide

Aldrich - I15602

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**MILLIPORE
SIGMA**

Formula : C₄H₇N
Molecular weight : 69.11 g/mol
CAS-No. : 78-82-0
EC-No. : 201-147-5

Component	Classification	Concentration
isobutyronitrile		
	Flam. Liq. 2; Acute Tox. 2; Aquatic Acute 3; H225, H300, H330, H310, 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. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

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. Remove contact lenses.

If swallowed

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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

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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

Nitrogen oxides (NO_x)

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

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

Forms explosive mixtures with air at ambient temperatures.

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. Suppress (knock down) gases/vapors/mists with a water spray jet. 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. Chemizorb®). 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 safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

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 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

Component	CAS-No.	Value	Control parameters	Basis
isobutyronitrile	78-82-0	TWA	8 ppm 22 mg/m ³	USA. NIOSH Recommended Exposure Limits

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). Safety glasses

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: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 120 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

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: liquid |
| b) Odor | bitter almond-like |
| c) Odor Threshold | No data available |
| d) pH | 6 |
| e) Melting point/freezing point | Melting point/range: -72 °C (-98 °F) - lit. |
| f) Initial boiling point and boiling range | 107 - 108 °C 225 - 226 °F - lit. |
| g) Flash point | 8 °C (46 °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: 12.7 %(V)
Lower explosion limit: 1.6 %(V) |
| k) Vapor pressure | 43.5 hPa at 25 °C (77 °F)
133 hPa at 54.4 °C(129.9 °F) |
| l) Vapor density | 2.4 |

- | | |
|--|--|
| m) Density | 0.77 g/cm ³ at 20 °C (68 °F) - lit. |
| Relative density | No data available |
| n) Water solubility | 0.24 g/l at 25 °C (77 °F) |
| o) Partition coefficient:
n-octanol/water | log Pow: 0.46 - (Lit.), Bioaccumulation is not expected. |
| p) Autoignition
temperature | No data available |
| q) Decomposition
temperature | No data available |
| r) Viscosity | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | No data available |

9.2 Other safety information

Relative vapor density	2.4
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SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

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:

Strong oxidizing agents
Strong acids
strong alkalis
strong reducing agents

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

various plastics

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 - 50 mg/kg

Remarks: (RTECS)

LC50 Inhalation - Rat - 4 h - 0.85 mg/l - vapor

Remarks: (External MSDS)

LD50 Dermal - Rabbit - 200 mg/kg

Remarks: (RTECS)

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Remarks: (National Toxicology Program)

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: TZ4900000

May cause cyanosis., Always have on hand a cyanide first-aid kit, together with proper instructions.

Systemic effects:

Shortness of breath
Headache
Dizziness
confusion
muscular weakness
vasodilation
Tremors
Convulsions

Damage to:

Liver

The following applies to cyanogen compounds/ nitriles in general: utmost caution! Release of hydrocyanic acid is possible - blockade of cellular respiration. Cardiovascular disorders, dyspnoea, unconsciousness.

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish LC50 - Pimephales promelas (fathead minnow) - > 102.1 mg/l - 96 h
Remarks: (External MSDS)

LC50 - Pimephales promelas (fathead minnow) - 245 mg/l - 48 h
Remarks: (External MSDS)

Toxicity to daphnia and other aquatic invertebrates NOEC - Daphnia magna (Water flea) - 94.3 mg/l - 48 h
Remarks: (External MSDS)

EC50 - Daphnia magna (Water flea) - > 94.3 mg/l - 48 h
Remarks: (External MSDS)

12.2 Persistence and degradability

No data available

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

Discharge into the environment must be avoided.

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 2284 Class: 3 (6.1) Packing group: II
Proper shipping name: Isobutyronitrile
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2284 Class: 3 (6.1) Packing group: II EMS-No: F-E, S-D
Proper shipping name: ISOBUTYRONITRILE

IATA

UN number: 2284 Class: 3 (6.1) Packing group: II
Proper shipping name: Isobutyronitrile

SECTION 15: Regulatory information

SARA 302 Components

isobutyronitrile

CAS-No.
78-82-0

Revision Date
2008-11-03

SARA 313 Components

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.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
isobutyronitrile	78-82-0	2008-11-03

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
isobutyronitrile	78-82-0	2008-11-03

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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