

## SAFETY DATA SHEET

Version 8.2  
Revision Date 09/14/2020  
Print Date 11/20/2020**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 Street  
ST. LOUIS MO 63103  
UNITED STATESTelephone : +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, Dermal (Category 3), H311  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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 statement(s)	
H225	Highly flammable liquid and vapor.
H300	Fatal if swallowed.
H311	Toxic in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
Precautionary statement(s)	
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.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
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.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P312	Call a POISON CENTER/ doctor if you feel unwell.
P322	Specific measures (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P361	Remove/ Take off immediately all contaminated clothing.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
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

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : 2-Methylpropionitrile  
2-Methylpropanenitrile  
Isopropyl cyanide

Formula : C<sub>4</sub>H<sub>7</sub>N  
Molecular weight : 69.11 g/mol  
CAS-No. : 78-82-0  
EC-No. : 201-147-5

Component	Classification	Concentration
<b>isobutyronitrile</b>		
	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.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Small (incipient) fires must be extinguished with alcohol resistant foam, dry chemical powder or carbon dioxide. Large amounts of water are ineffective. Cool containers with large amounts of water.

## **5.2 Special hazards arising from the substance or mixture**

Carbon oxides, Nitrogen oxides (NO<sub>x</sub>)

## **5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

## **5.4 Further information**

Use water spray to cool unopened containers.

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## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

### **6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### **6.3 Methods and materials for containment and cleaning up**

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

### **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

### **7.2 Conditions for safe storage, including any incompatibilities**

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

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

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## **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/m3	USA. NIOSH Recommended Exposure Limits

## 8.2 Exposure controls

### Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

### Personal protective equipment

#### Eye/face protection

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

#### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: > 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: > 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

#### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: clear, liquid Color: colorless
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
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	No data available
k) Vapor pressure	No data available
l) Vapor density	2.39 - (Air = 1.0)
m) Relative density	0.77 g/cm <sup>3</sup> at 20 °C (68 °F)
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
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	2.39 - (Air = 1.0)
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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

## 10.2 Chemical stability

Stable under recommended storage conditions.

## 10.3 Possibility of hazardous reactions

Vapors may form explosive mixture with air.

## 10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

## 10.5 Incompatible materials

Strong acids, Strong bases, Strong oxidizing agents, Strong reducing agents

## 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>)

Other decomposition products - No data available

In the event of fire: see section 5

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## 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

Remarks: (External MSDS)

LD50 Dermal - Rabbit - 200 mg/kg

Remarks: (RTECS)

#### Skin corrosion/irritation

#### Serious eye damage/eye irritation

#### Respiratory or skin sensitization

#### Germ cell mutagenicity

Ames test

Salmonella typhimurium

Result: negative

(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.

ACGIH: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

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

## Specific target organ toxicity - single exposure

## Specific target organ toxicity - repeated exposure

## Aspiration hazard

## 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.

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## 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

### 12.3 Bioaccumulative potential

### 12.4 Mobility in soil

### 12.5 Results of PBT and vPvB assessment

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

### 12.6 Other adverse effects

Discharge into the environment must be avoided.



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**SECTION 13: Disposal considerations****13.1 Waste treatment methods****Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. 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.

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**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

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**SECTION 15: Regulatory information****SARA 302 Components**

The following components are subject to reporting levels established by SARA Title III, Section 302:

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

isobutyronitrile	CAS-No. 78-82-0	Revision Date 2008-11-03
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**Pennsylvania Right To Know Components**

isobutyronitrile	CAS-No. 78-82-0	Revision Date 2008-11-03
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## New Jersey Right To Know Components

isobutyronitrile

CAS-No.  
78-82-0

Revision Date  
2008-11-03

## California Prop. 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

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### SECTION 16: Other information

#### Further information

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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](http://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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