

SAFETY DATA SHEET

Revision Date 18-Dec-2025

Revision Number 6

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

Product Name	Isobutyronitrile
Cat No. :	AC122530000; AC122530010; AC122530050
CAS No	78-82-0
Synonyms	2-Methylpropionitrile; Isopropyl cyanide
Recommended Use	Laboratory chemicals.
Uses advised against	Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024).

Flammable liquids	Category 2
Acute oral toxicity	Category 2
Acute dermal toxicity	Category 3
Acute Inhalation Toxicity - Vapors	Category 2
Specific target organ toxicity (single exposure)	Category 2

Label Elements

Signal Word

Signal Danger

Hazard Statements

Hazard statements

Toxic in contact with skin
May cause damage to organs
Fatal if swallowed or if inhaled



Precautionary Statements

Prevention

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Wear protective gloves/protective clothing/eye protection/face protection
Do not breathe dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Wear respiratory protection
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
Keep container tightly closed
Ground and bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Keep cool
Take action to prevent static discharges
Use non-sparking tools

Response

IF exposed or concerned: Call a POISON CENTER or doctor

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing
Immediately call a POISON CENTER or doctor

Skin

Call a POISON CENTER or doctor if you feel unwell
Take off contaminated clothing and wash before reuse
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

Ingestion

IF SWALLOWED: Immediately call a POISON CENTER or doctor
Rinse mouth

Fire

In case of fire: Use CO₂, dry chemical, or foam to extinguish

Storage

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

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

3. Composition/information on Ingredients

Component	CAS No	Weight %
Isobutyronitrile	78-82-0	99

4. First-aid measures

Eye Contact	Immediate medical attention is required. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.
Skin Contact	Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention. Take off contaminated clothing and shoes immediately.
Inhalation	Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Immediate medical attention is required.
Ingestion	Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Drink plenty of water. Call a physician immediately. If possible drink milk afterwards.
Most important symptoms and effects	Difficulty in breathing. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray. Carbon dioxide (CO ₂). Dry chemical. Alcohol resistant foam. Use extinguishing measures that are appropriate to local circumstances and the surrounding environment. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	8 °C / 46.4 °F
Method -	No information available
Autoignition Temperature	482 °C / 899.6 °F
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

Hazardous Combustion Products

Nitrogen oxides (NO_x). Thermal decomposition can lead to release of irritating gases and vapors. Carbon monoxide (CO). Carbon dioxide (CO₂).

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
4	3	0	N/A

6. Accidental release measures

Personal Precautions	Remove all sources of ignition. Take precautionary measures against static discharges.
Environmental Precautions	See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Sweep up and shovel into suitable containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

7. Handling and Storage

Handling

Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

Storage.

Flammables area. Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Keep container tightly closed in a dry and well-ventilated place. Keep away from heat, sparks and flame. Incompatible Materials. Strong oxidizing agents. Strong acids. Strong bases. Strong reducing agents. Oxidizing agent.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
Isobutyronitrile		(Vacated) TWA: 5 mg/m ³	IDLH: 25 mg/m ³ REL = 8 ppm (TWA) REL = 22 mg/m ³ (TWA)	

Legend

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ventilation systems. Use explosion-proof electrical/ventilating/lighting equipment.

Personal Protective Equipment

Eye/face Protection

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection

Wear a NIOSH/MSHA or European Standard EN 149 approved full-facepiece airline respirator in the positive pressure mode with emergency escape provisions.

Recommended Filter type:

Organic gases and vapours filter. Type A. Brown. conforming to EN14387.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance

Physical State

Liquid

Color

Light yellow

Odor

bitter almonds

Odor Threshold

No information available

Property

Values

-72 °C / -97.6 °F

Remarks

• Method

Melting Point/Range

Softening Point	No data available	
Boiling Point/Range	107 - 108 °C / 224.6 - 226.4 °F	@ 760 mmHg
Flash Point	8 °C / 46.4 °F	Method - No information available
Flammability (liquid)	Highly flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Autoignition Temperature	482 °C / 899.6 °F	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	35 g/l (20 C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)	log Pow	
Component	0.46	
Isobutyronitrile		
Vapor Pressure	100 mmHg @ 54.4 °C	
Density / Specific Gravity	0.760	
Bulk Density	Not applicable	Liquid
Vapor Density	2.4	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	
Other Information		
Molecular Formula	C4 H7 N	
Molecular Weight	69.11	
Explosive Properties	Vapors may form explosive mixtures with air	

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.
Incompatible Materials	Strong oxidizing agents, Strong acids, Strong bases, Strong reducing agents, Oxidizing agent
Hazardous Decomposition Products	Nitrogen oxides (NOx), Thermal decomposition can lead to release of irritating gases and vapors, Carbon monoxide (CO), Carbon dioxide (CO ₂)
Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation	Not an expected route of exposure.
Ingestion	May be harmful if swallowed.
Eyes	Avoid contact with eyes.
Skin	Avoid contact with skin. Harmful in contact with skin.

Toxicology data for the components

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isobutyronitrile	LD50 = 50 mg/kg (Rat)	LD50 = 310 mg/kg (Rabbit)	LC50 > 3.4 mg/L (Rat) 1 h

Toxicologically Synergistic Products No information available

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;
 Respiratory No data available
 Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity;

The table below indicates whether each agency has listed any ingredient as a carcinogen

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Isobutyronitrile	78-82-0	Not listed				

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects,both acute and delayed Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting.

Other Adverse Effects The toxicological properties have not been fully investigated.

Endocrine Disrupting Properties This product does not contain any known or suspected endocrine disruptors.

12. Ecological information

Ecotoxicity

Persistence and Degradability Persistence is unlikely

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its water solubility.

Component	log Pow
Isobutyronitrile	0.46

13. Disposal considerations

Waste Disposal Methods	Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.
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14. Transport information

DOT

UN-No	UN2284
Hazard Class	3
Subsidiary Hazard Class	6.1
Packing Group	II

TDG

UN-No	UN2284
Hazard Class	3
Subsidiary Hazard Class	6.1
Packing Group	II

IATA

UN-No	UN2284
Proper Shipping Name	ISOBUTYRONITRILE
Hazard Class	3
Subsidiary Hazard Class	6.1
Packing Group	II

IMDG/IMO

UN-No	UN2284
Proper Shipping Name	ISOBUTYRONITRILE
Hazard Class	3
Subsidiary Hazard Class	6.1
Packing Group	II

15. Regulatory Information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Isobutyronitrile	78-82-0	X	ACTIVE	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Isobutyronitrile	78-82-0	-	X	201-147-5	X	X	X	X	X	KE-24871

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations

SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product contains a chemical or chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372.

Component	CAS No	Weight %	SARA 313 - Threshold Values %	SARA 313 - Reporting thresholds
Isobutyronitrile	78-82-0	99	1.0 %	-

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act)

Component	CWA - Hazardous Substances	CWA - Reportable Quantities	CWA - Toxic Pollutants	CWA - Priority Pollutants
Isobutyronitrile	-	-	X	X

Clean Air Act

Component	HAPS Data	Class 1 Ozone Depletors	Class 2 Ozone Depletors
Isobutyronitrile	X		-

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355).

Component	Hazardous Substances RQs	CERCLA Extremely Hazardous Substances RQs	SARA Reportable Quantity (RQ)
Isobutyronitrile	-	1000 lb	-

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Isobutyronitrile	X	X	X	X	X

U.S. Department of Transportation

Reportable Quantity (RQ): N
 DOT Marine Pollutant Y
 DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product contains the following DHS chemicals:
Legend - STQs = Screening Threshold Quantities, APA = A placarded amount

Component	DHS Chemical Facility Anti-Terrorism Standard
Isobutyronitrile	Release STQs - 20000lb

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances	REACH (1907/2006) - Annex XVII - Restrictions	REACH Regulation (EC 1907/2006) article 59 -

		Subject to Authorization	on Certain Dangerous Substances	Candidate List of Substances of Very High Concern (SVHC)
Isobutyronitrile	78-82-0	-	-	-

Safety, health and environmental regulations/legislation specific for the substance or mixture

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Isobutyronitrile	78-82-0	Listed	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Isobutyronitrile	78-82-0	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information**Prepared By**

Product stewardship (Regulatory Affairs)
 Thermo Fisher Scientific
 email - begel.sdsdesk@thermofisher.com

Revision Date

18-Dec-2025

Print Date

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Revision Summary

Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS