

# SAFETY DATA SHEET

Creation Date 13-Oct-2009

Revision Date 19-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** Isovaleronitrile

**Cat No. :** AC427560000; AC427560050; AC427560250

**CAS No** 625-28-5  
**Synonyms** 3-Methylbutyronitrile; 3-Methylbutanenitrile

**Recommended Use** Laboratory chemicals.  
**Uses advised against** Food, drug, pesticide or biocidal product use.

### Details of the supplier of the safety data sheet

#### Company

Fisher Scientific Company  
One Reagent Lane  
Fair Lawn, NJ 07410  
Tel: (201) 796-7100

Acros Organics  
One Reagent Lane  
Fair Lawn, NJ 07410

#### **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 3
Acute oral toxicity	Category 3
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

### Label Elements

**Signal Word**  
Danger

**Hazard Statements**

Flammable liquid and vapor  
Toxic if swallowed  
Causes skin irritation  
Causes serious eye irritation  
May cause respiratory irritation

**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  
Avoid breathing dust/fume/gas/mist/vapors/spray  
Use only outdoors or in a well-ventilated area  
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

**Inhalation**

IF INHALED: Remove person to fresh air and keep comfortable for breathing  
Call a POISON CENTER or doctor if you feel unwell

**Skin**

If skin irritation occurs: Get medical advice/attention  
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower  
Take off contaminated clothing and wash before reuse

**Eyes**

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
If eye irritation persists: Get medical advice/attention

**Ingestion**

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

**Fire**

In case of fire: Use CO<sub>2</sub>, 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 %
Butanenitrile, 3-methyl-	625-28-5	>95

#### 4. First-aid measures

<b>General Advice</b>	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Inhalation</b>	Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately.
<b>Most important symptoms and effects</b>	. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
<b>Notes to Physician</b>	Treat symptomatically

#### 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Water spray, carbon dioxide (CO <sub>2</sub> ), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.
<b>Unsuitable Extinguishing Media</b>	No information available
<b>Flash Point</b>	28 °C / 82.4 °F
<b>Method -</b>	No information available
<b>Autoignition Temperature</b>	No information available
<b>Explosion Limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Sensitivity to Mechanical Impact</b>	No information available
<b>Sensitivity to Static Discharge</b>	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

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Nitrogen oxides (NO<sub>x</sub>).

#### 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. Thermal decomposition can lead to release of irritating gases and vapors.

#### NFPA

<b>Health</b>	<b>Flammability</b>	<b>Instability</b>	<b>Physical hazards</b>
3	3	0	N/A

## 6. Accidental release measures

<b>Personal Precautions</b>	Use personal protective equipment as required. Ensure adequate ventilation. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas. Remove all sources of ignition. Take precautionary measures against static discharges.
<b>Environmental Precautions</b>	Should not be released into the environment.
<b>Methods for Containment and Clean Up</b>	Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

## 7. Handling and Storage

<b>Handling</b>	Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.
<b>Storage.</b>	Keep container tightly closed in a dry and well-ventilated place. Flammables area. Keep away from heat, sparks and flame. To maintain product quality. Keep refrigerated. Incompatible Materials. Strong oxidizing agents.

## 8. Exposure controls / personal protection

### Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
Butanenitrile, 3-methyl-		(Vacated) TWA: 5 mg/m <sup>3</sup>	IDLH: 25 mg/m <sup>3</sup>	

### Legend

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

<b>Engineering Measures</b>	Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting equipment. Ensure adequate ventilation, especially in confined areas.
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### Personal Protective Equipment

<b>Eye/face Protection</b>	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.
<b>Skin and body protection</b>	Wear appropriate protective gloves and clothing to prevent skin exposure.
<b>Respiratory Protection</b>	Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
<b>Recommended Filter type:</b>	Organic gases and vapours filter. Type A. Brown. conforming to EN14387.
<b>Hygiene Measures</b>	Handle in accordance with good industrial hygiene and safety practice.

## 9. Physical and chemical properties

### Appearance

<b>Physical State</b>	Liquid		
<b>Color</b>	Clear, Colourless		
<b>Odor</b>	No information available		
<b>Odor Threshold</b>	No information available		
<b>Property</b>	<b>Values</b>	<b>Remarks</b>	<b>• Method</b>
<b>Melting Point/Range</b>	No data available		
<b>Softening Point</b>	No data available		
<b>Boiling Point/Range</b>	128 - 130 °C / 262.4 - 266 °F	@ 730 mmHg	
<b>Flash Point</b>	28 °C / 82.4 °F		
<b>Flammability (liquid)</b>	Flammable	<b>Method -</b> No information available	
<b>Flammability (solid,gas)</b>	Not applicable	On basis of test data	
<b>Explosion Limits</b>	No data available	Liquid	
<b>Autoignition Temperature</b>	No data available		
<b>Decomposition Temperature</b>	No data available		
<b>pH</b>	No information available		
<b>Viscosity</b>	No data available		
<b>Water Solubility</b>	No information available		
<b>Solubility in other solvents</b>	No information available		
<b>Partition Coefficient (n-octanol/water)</b>			
<b>Vapor Pressure</b>	No data available		
<b>Density / Specific Gravity</b>	0.795		
<b>Bulk Density</b>	Not applicable	Liquid	
<b>Vapor Density</b>	No data available	(Air = 1.0)	
<b>Particle characteristics</b>	Not applicable (liquid)		
<b>Other Information</b>			
<b>Molecular Formula</b>	C5 H9 N		
<b>Molecular Weight</b>	83.13		
<b>Explosive Properties</b>	explosive air/vapour mixtures possible		

## 10. Stability and reactivity

<b>Reactive Hazard</b>	None known, based on information available
<b>Stability</b>	Stable under normal conditions.
<b>Conditions to Avoid</b>	Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.
<b>Incompatible Materials</b>	Strong oxidizing agents
<b>Hazardous Decomposition Products</b>	Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> ), Nitrogen oxides (NO <sub>x</sub> )
<b>Hazardous Polymerization</b>	Hazardous polymerization does not occur.
<b>Hazardous Reactions</b>	None under normal processing.

## 11. Toxicological information

### Information on expected route of exposure

<b>Inhalation</b>	Harmful by inhalation. Irritating to respiratory system.
<b>Ingestion</b>	Harmful if swallowed. Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhea.
<b>Eyes</b>	Irritating to eyes.
<b>Skin</b>	Harmful in contact with skin. Irritating to skin.

### Toxicology data for the components

**Toxicologically Synergistic Products** No information available

**(b) skin corrosion/irritation;** Category 2

**(c) serious eye damage/irritation;** Category 2

**(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
Butanenitrile, 3-methyl-	625-28-5	Not listed	Not listed	Not listed	Not listed	Not listed

**(g) reproductive toxicity;** No data available

**(h) STOT-single exposure;** Category 3  
**Results / Target organs** Respiratory system.

**(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** Symptoms of overexposure may be 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

Do not empty into drains.

**Persistence and Degradability** No information available

**Bioaccumulation/ Accumulation** No information available.

**Mobility** No information available.

### 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.

### 14. Transport information

**DOT**

**UN-No** UN1992  
**Proper Shipping Name** Flammable liquid, toxic, n.o.s.  
**Technical Shipping Name** Butanenitrile, 3-methyl-  
**Hazard Class** 3  
**Subsidiary Hazard Class** 6.1  
**Packing Group** III

**TDG**

**UN-No** UN1992  
**Proper Shipping Name** Flammable liquid, toxic, n.o.s.  
**Technical Shipping Name** Butanenitrile, 3-methyl-  
**Hazard Class** 3  
**Subsidiary Hazard Class** 6.1  
**Packing Group** III

**IATA**

**UN-No** UN1992  
**Proper Shipping Name** Flammable liquid, toxic, n.o.s.  
**Technical Shipping Name** Butanenitrile, 3-methyl-  
**Hazard Class** 3  
**Subsidiary Hazard Class** 6.1  
**Packing Group** III

**IMDG/IMO**

**UN-No** UN1992  
**Proper Shipping Name** Flammable liquid, toxic, n.o.s.  
**Technical Shipping Name** Butanenitrile, 3-methyl-  
**Hazard Class** 3  
**Subsidiary Hazard Class** 6.1  
**Packing Group** III

### 15. Regulatory Information

**United States of America Inventory**

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Butanenitrile, 3-methyl-	625-28-5	X	INACTIVE	-

**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
Butanenitrile, 3-methyl-	625-28-5	-	X	210-884-1	-	-		X	X	KE-09093

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
Butanenitrile, 3-methyl-	625-28-5	>95	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
Butanenitrile, 3-methyl-	-	-	X	X

#### Clean Air Act

Component	HAPS Data	Class 1 Ozone Depletors	Class 2 Ozone Depletors
Butanenitrile, 3-methyl-	X		-

OSHA - Occupational Safety and Health Administration Not applicable

#### CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

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
Butanenitrile, 3-methyl-	-	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 does not contain any DHS chemicals.

#### Other International Regulations

Mexico - Grade Serious risk, Grade 3

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) -	REACH (1907/2006) -	REACH Regulation (EC)

		Annex XIV - Substances Subject to Authorization	Annex XVII - Restrictions on Certain Dangerous Substances	1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Butanenitrile, 3-methyl-	625-28-5	-	-	-

#### 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)
Butanenitrile, 3-methyl-	625-28-5	Not applicable	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)
Butanenitrile, 3-methyl-	625-28-5	Not applicable	Not applicable	Not applicable	Not applicable

## 16. Other Information

<b>Prepared By</b>	Product stewardship (Regulatory Affairs) Thermo Fisher Scientific email - begel.sdsdesk@thermofisher.com
<b>Creation Date</b>	13-Oct-2009
<b>Revision Date</b>	19-Dec-2025
<b>Print Date</b>	19-Dec-2025
<b>Revision Summary</b>	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**