

SAFETY DATA SHEET

Creation Date 13-Oct-2009

Revision Date 26-Dec-2021

Revision Number 5

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-ACROS-01 / **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 by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

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/sparks/open flames/hot surfaces. - No smoking
 Keep container tightly closed
 Ground/bond container and receiving equipment
 Use explosion-proof electrical/ventilating/lighting equipment
 Use only non-sparking tools
 Take precautionary measures against static discharge
 Keep cool

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
 Call a POISON CENTER or doctor/physician 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/shower
 Wash contaminated clothing 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/physician
 Rinse mouth

Fire

In case of fire: Use CO₂, dry chemical, or foam for extinction

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

3. Composition/Information on Ingredients

Component	CAS No	Weight %
Butanenitrile, 3-methyl-	625-28-5	>95

4. First-aid measures

General Advice	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
Eye Contact	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.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
Inhalation	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.
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.
Most important symptoms and effects	. Symptoms of overexposure may be 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. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	28 °C / 82.4 °F
Method -	No information available
Autoignition Temperature	No information available
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

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x).

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

Health
3

Flammability
3

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions	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.
Environmental Precautions	Should not be released into the environment.

Methods for Containment and Clean Up 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

Handling 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.

Storage. 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 IDLH	Mexico OEL (TWA)
Butanenitrile, 3-methyl-		(Vacated) TWA: 5 mg/m ³	IDLH: 25 mg/m ³	

Legend

OSHA - Occupational Safety and Health Administration

NIOSH IDLH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures 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.

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 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.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Clear, Colourless
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	No data available
Boiling Point/Range	128 - 130 °C / 262.4 - 266 °F @ 730 mmHg
Flash Point	28 °C / 82.4 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	

Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	No information available
Specific Gravity	0.795
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C5 H9 N
Molecular Weight	83.13

10. Stability and reactivity

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

11. Toxicological information

Acute Toxicity

Product Information

Component Information

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	Irritating to eyes, respiratory system and skin
Sensitization	No information available
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

Mutagenic Effects	No information available
Reproductive Effects	No information available.
Developmental Effects	No information available.
Teratogenicity	No information available.
STOT - single exposure	Respiratory system
STOT - repeated exposure	None known
Aspiration hazard	No information available

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Endocrine Disruptor Information No information available

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

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 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.
Hazard Class 3
Subsidiary Hazard Class 6.1
Packing Group III

IATA

UN-No UN1992
Proper Shipping Name Flammable liquid, toxic, n.o.s.
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.
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 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

Component	CAS No	Weight %	SARA 313 - Threshold Values %
Butanenitrile, 3-methyl-	625-28-5	>95	1.0

SARA 311/312 Hazard Categories See section 2 for more information

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 Not applicable

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

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

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

Prepared By	Regulatory Affairs Thermo Fisher Scientific Email: EMSDS.RA@thermofisher.com
Creation Date	13-Oct-2009
Revision Date	26-Dec-2021
Print Date	26-Dec-2021
Revision Summary	This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

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