SAFETY DATA SHEET according to the OSHA Hazard Communication Standard

Version 6.10
Revision Date 07/10/2026
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Isovaleric acid

Product Number : W310212
Brand : Aldrich
CAS-No. : 503-74-2

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

Identified uses : Laboratory chemicals, Synthesis of substances

Restrictions on use : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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 number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Flammable liquids : Category 4

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Skin corrosion	:	Sub-category 1B
Serious eye damage	:	Category 1
Short-term (acute) aquatic hazard	:	Category 3

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements : H227 Combustible liquid.
H314 Causes severe skin burns and eye damage.
H402 Harmful to aquatic life.

Precautionary statements :

Prevention:

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P264 Wash skin thoroughly after handling.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response:

P301 + P330 + P331 + P310 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. Immediately call a POISON CENTER/ doctor.
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.
P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P363 Wash contaminated clothing before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

Storage:

P403 Store in a well-ventilated place.
P405 Store locked up.

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Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 503-74-2

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
3-methylbutyric acid	503-74-2*	>= 80 - <= 100	TSC

* Indicates that the identifier is a CAS No.
TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : First aiders need to protect themselves.
Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air. Call in physician.

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.
Immediately call in ophthalmologist.
Remove contact lenses.

If swallowed : After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation).
Call a physician immediately.
Do not attempt to neutralise.

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

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

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SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	:	Carbon dioxide (CO2) Foam Dry powder
Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	:	Combustible. Vapours are heavier than air and may spread along floors. Forms explosive mixtures with air on intense heating. Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	:	Carbon oxides
Specific extinguishing methods	:	No data available
Further information	:	Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	:	Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	:	Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

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		Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	:	Do not let product enter drains.
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 with liquid-absorbent and neutralising material (e.g. Chemizorb® H^+, Merck Art. No. 101595). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	:	Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Further information on storage conditions	:	Tightly closed. Keep locked up or in an area accessible only to qualified or authorised persons.
Storage class	:	8A, Combustible, corrosive hazardous materials
Recommended storage temperature	:	Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

Respiratory protection	:	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.

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Recommended Filter type:	:	Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepeneur 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.

Hand protection

Material	:	butyl-rubber
Break through time	:	480 min
Glove thickness	:	0.7 mm
Protective index	:	Full contact
Manufacturer	:	Butoject® (KCL 898)
Material	:	Nitrile rubber
Break through time	:	240 min
Glove thickness	:	0.4 mm
Protective index	:	Splash contact
Manufacturer	:	Camatril® (KCL 730 / Aldrich Z677442, Size M)
Remarks	:	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).

Eye protection	:	Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles
Skin and body protection	:	protective clothing
Hygiene measures	:	Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	:	liquid (68 °F / 20 °C, 1,013 hPa)
Colour	:	colourless

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Odour	:	unpleasant
Odour Threshold	:	No data available
pH	:	3.1 (77 °F / 25 °C) Concentration: 10 g/l Method: DIN 19268
Melting point/ range	:	ca. -24 °F / -31 °C Method: OECD Test Guideline 102
Boiling point/boiling range	:	353.3 °F / 178.5 °C (1,013 hPa) Method: OECD Test Guideline 103
Flash point	:	176 °F / 80 °C (1,013 hPa) Method: ISO 2719, Pensky-Martens closed cup
Evaporation rate	:	No data available
Flammability (solid, gas)	:	No data available
Flammability (liquids)	:	No data available
Burning rate	:	No data available
Self-ignition	:	788 °F / 420 °C 988 hPa Method: Tested according to Directive 92/69/EEC. GLP: yes
Upper explosion limit / Upper flammability limit	:	Upper explosion limit 6.8 %(V)
Lower explosion limit / Lower flammability limit	:	Lower explosion limit 1.5 %(V)
Vapour pressure	:	ca. 1 hPa (68 °F / 20 °C)
Relative vapour density	:	No data available
Relative density	:	No data available
Density	:	0.93 g/cm3 (68 °F / 20 °C) Method: OECD Test Guideline 109
Solubility(ies)		
Water solubility	:	48 g/l completely soluble (68 °F / 20 °C) pH: 2.4 Method: OECD Test Guideline 105 GLP: yes

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Partition coefficient: n-octanol/water	:	Pow: 50 (77 °F / 25 °C) log Pow: 1.7 (77 °F / 25 °C) pH: 3 Method: OECD Test Guideline 117 GLP: yes Bioaccumulation is not expected.
Autoignition temperature	:	788 °F / 420 °C (988 hPa) Method: Tested according to Directive 92/69/EEC. GLP: yes
Decomposition temperature	:	> 572 °F / > 300 °C
Viscosity		
Viscosity, dynamic	:	2.437 mPa.s (68 °F / 20 °C) Method: ASTM D 445
Viscosity, kinematic	:	No data available
Flow time	:	No data available
Explosive properties	:	Not classified as explosive.
Oxidizing properties	:	none
Surface tension	:	63.3 mN/m, 1 g/l, 68 °F / 20 °C, OECD Test Guideline 115, GLP: yes
Molecular weight	:	102.13 g/mol
Particle characteristics		
Particle size	:	No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	:	Forms explosive mixtures with air on intense heating. A range from approx. 15 Kelvin below the flash point is to be rated as critical.
Chemical stability	:	The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	:	Violent reactions possible with: alkalines Amines Nitriles Oxidizing agents

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Conditions to avoid	:	Strong heating.
Incompatible materials	:	No data available
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 - male and female - 2,500 mg/kg
(OECD Test Guideline 401)
Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the oesophagus and the stomach.
Inhalation: Corrosive to respiratory system.
Inhalation: Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.
Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract
Dermal: No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Corrosive - 3 min - 1 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Remarks: Causes serious eye damage.

Respiratory or skin sensitization
No data available

Germ cell mutagenicity

Test Type: Micronucleus test
Species: Mouse
Cell type: Red blood cells (erythrocytes)
Application Route: Oral
Method: OECD Test Guideline 474
Result: negative
Remarks: The value is given in analogy to the following substances: Isoamyl alcohol

Carcinogenicity

IARC: No component 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 component 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

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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

Repeated dose toxicity - Rat - male - Oral - 90 Days - No observed adverse effect level - 5,000 mg/kg
Remarks: (ECHA)
The value is given in analogy to the following substances: Sodium isovalerate-1-13C

RTECS: NY1400000
Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Inhalation may provoke the following symptoms:, spasm, inflammation and edema of the bronchi, spasm, inflammation and edema of the larynx, pneumonitis, pulmonary edema, Symptoms and signs of poisoning are:, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

3-methylbutyric acid:

Toxicity to fish	:	LC50 (Pimephales promelas (fathead minnow)): 77 mg/l End point: mortality Exposure time: 96 h Test Type: static test Method: OECD Test Guideline 203 Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: valeric acid
Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Daphnia magna (Water flea)): 51.25 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Method: OECD Test Guideline 202

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Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: 2-methylpropionic acid; isobutyric acid

Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata): 29.3 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: valeric acid

NOEC (Pseudokirchneriella subcapitata): 6.38 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: valeric acid

Toxicity to microorganisms : EC0 (activated sludge): > 1,000 mg/l
Test Type: fermentation tube test
Remarks: (External MSDS)

Persistence and degradability

Components:

3-methylbutyric acid:

Biodegradability : aerobic
Inoculum: activated sludge
Concentration: 100 mg/l
Result: Readily biodegradable.
Biodegradation: 58 - 66 %
Exposure time: 10 d
Method: OECD Test Guideline 301C

Bioaccumulative potential

Components:

3-methylbutyric acid:

Partition coefficient: n-octanol/water : Pow: 50 (77 °F / 25 °C)
log Pow: 1.7 (77 °F / 25 °C)
pH: 3

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Method: OECD Test Guideline 117
GLP: yes
Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Components:

3-methylbutyric acid:

Additional ecological information : Discharge into the environment must be avoided.

Endocrine disrupting properties

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No.	:	UN 3265
Proper shipping name	:	Corrosive liquid, acidic, organic, n.o.s. (3-methylbutyric acid)
Class	:	8
Packing group	:	II
Labels	:	Class 8 - Corrosive substances
Packing instruction (cargo aircraft)	:	855
Packing instruction	:	851

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(passenger aircraft)

IMDG-Code

UN number	:	UN 3265
Proper shipping name	:	CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (3-methylbutyric acid)
Class	:	8
Packing group	:	II
Labels	:	8
EmS Code	:	F-A, S-B
Marine pollutant	:	no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

UN/ID/NA number	:	UN 3265
Proper shipping name	:	Corrosive liquid, acidic, organic, n.o.s. (3-methylbutyric acid)
Class	:	8
Packing group	:	II
Labels	:	Class 8 - Corrosive substances
ERG Code	:	153
Marine pollutant	:	no
Poison Inhalation Hazard	:	No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards	:	Fire Hazard Acute Health Hazard

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SARA 313 : 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.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).
This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).
This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).
This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCMI Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.
This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.
This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307
This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

3-methylbutyric acid	503-74-2

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

US TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

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AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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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