SAFETY DATA SHEET

Version 6.7
Revision Date 08/31/2021
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Isovaleric acid

Product Number : 129542
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

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

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 4), H227
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Short-term (acute) aquatic hazard (Category 3), H402

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

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Hazard statement(s)	
H227	Combustible liquid.
H314	Causes severe skin burns and eye damage.
H402	Harmful to aquatic life.

Precautionary statement(s)	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P264	Wash skin thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
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.
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

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms	:	3-Methylbutanoic acid 3-Methylbutyric acid
Formula	:	$C_5H_{10}O_2$
Molecular weight	:	102.13 g/mol
CAS-No.	:	503-74-2
EC-No.	:	207-975-3

Component	Classification	Concentration
3-methylbutyric acid		
	Flam. Liq. 4; Skin Corr. 1B; Eye Dam. 1; Aquatic Acute 3; H227, H314, H318, 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
Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.Continue rinsing eyes during transport to hospital.

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Unsuitable extinguishing media
Do NOT use water jet.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Combustible.

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.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of

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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. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling
Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion
Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.

Hygiene measures
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
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
Storage class (TRGS 510): 8A: Combustible, corrosive hazardous materials

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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Personal protective equipment

Eye/face protection
Tightly fitting safety goggles. Faceshield (8-inch minimum). 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: Nitrile rubber
Minimum layer thickness: 0.2 mm
Break through time: 30 min
Material tested:Dermatril® P (KCL 743 / Aldrich Z677388, 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, 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. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid Color: colorless
b)	Odor	unpleasant

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c)	Odor Threshold	No data available
d)	pH	3.1 at 10 g/l at 25 °C (77 °F) - DIN 19268
e)	Melting point/freezing point	Melting point: ca.-31 °C (ca.-24 °F) - OECD Test Guideline 102
f)	Initial boiling point and boiling range	178.5 °C 353.3 °F at 1,013 hPa - OECD Test Guideline 103
g)	Flash point	80 °C (176 °F) - Pensky-Martens closed cup - ISO 2719
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 6.8 %(V) Lower explosion limit: 1.5 %(V)
k)	Vapor pressure	ca.1 hPa at 20 °C (68 °F)
l)	Vapor density	No data available
m)	Density	0.93 g/cm3 at 20 °C (68 °F) - OECD Test Guideline 109
	Relative density	No data available
n)	Water solubility	48 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - completely soluble
o)	Partition coefficient: n-octanol/water	Pow: 50; log Pow: 1.7 at 25 °C (77 °F) - Bioaccumulation is not expected.
p)	Autoignition temperature	420 °C (788 °F) at 988 hPa - Tested according to Directive 92/69/EEC.
q)	Decomposition temperature	> 300 °C (> 572 °F) -
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	none

9.2 Other safety information

Surface tension	63.3 mN/m at 1g/l at 20 °C (68 °F) - OECD Test Guideline 115
Dissociation constant	4.7 at 20.1 °C (68.2 °F) - OECD Test Guideline 112

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
No data available

10.4 Conditions to avoid
Heat, flames and sparks.

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10.5 Incompatible materials
Bases, Oxidizing agents, Reducing agents

10.6 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 esophagus and the stomach.
LC0 Inhalation - Rat - 4 h - 2.48 mg/l
(OECD Test Guideline 403)
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
Inhalation: Corrosive to respiratory system.
Dermal: No data available
No data available

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

Serious eye damage/eye irritation
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: (in analogy to similar products)

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.

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
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 - NOAEL (No observed adverse effect level) - 5,000 mg/kg
Remarks: (in analogy to similar products)
(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

12.1 Toxicity

Toxicity to fish	static test LC50 - Pimephales promelas (fathead minnow) - 77 mg/l - 96 h (OECD Test Guideline 203) Remarks: (in analogy to similar products) The value is given in analogy to the following substances: valeric acid
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 51.25 mg/l - 48 h (OECD Test Guideline 202) Remarks: (in analogy to similar products) The value is given in analogy to the following substances: 2-methylpropionic acid; isobutyric acid
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - 29.3 mg/l - 72 h (OECD Test Guideline 201) Remarks: (in analogy to similar products) The value is given in analogy to the following substances: valeric acid
	static test NOEC - Pseudokirchneriella subcapitata - 6.38 mg/l - 72 h (OECD Test Guideline 201)

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Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: valeric acid

Toxicity to bacteria — static test IC50 - Tetrahymena pyriformis - 224 mg/l - 40 h
Remarks: (ECHA)

fermentation tube test EC0 - activated sludge - > 1,000 mg/l
Remarks: (External MSDS)

12.2 Persistence and degradability

Biodegradability — aerobic - Exposure time 10 d
Result: 58 - 66 % - Readily biodegradable.
(OECD Test Guideline 301C)

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

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

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Harmful to aquatic life.
Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 3265 Class: 8 Packing group: II
Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (3-methylbutyric acid)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 3265 Class: 8 Packing group: II EMS-No: F-A, S-B

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Proper shipping name: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (3-methylbutyric acid)

IATA
UN number: 3265 Class: 8 Packing group: II
Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (3-methylbutyric acid)

SECTION 15: Regulatory information

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

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

	CAS-No.	Revision Date
3-methylbutyric acid	503-74-2	1993-04-24

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
3-methylbutyric acid	503-74-2	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
3-methylbutyric acid	503-74-2	1993-04-24

SECTION 16: Other information

Further information
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