

SAFETY DATA SHEET

Version 6.8
Revision Date 10/27/2023
Print Date 12/09/2023

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Isovaleric acid

Product Number : 129542
Brand : CCS
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 : Consolidated Chemicals & Solvents LLC
405 Business park lane
Allentown PA 18109
UNITED STATES

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

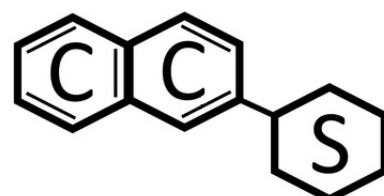
GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

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
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

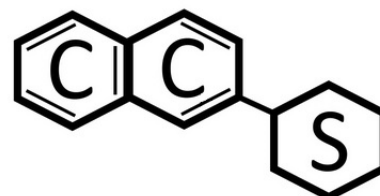
3.1 Substances

Synonyms : 3-Methylbutanoic acid
3-Methylbutyric acid

Formula : C₅H₁₀O₂
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.



SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

First aiders need to protect themselves. Show this material 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.

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

Carbon dioxide (CO₂) Foam Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

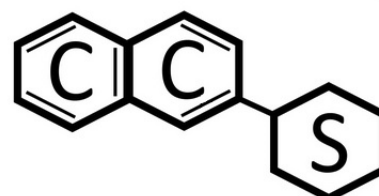
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.



SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 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.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

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

7.3 Specific end use(s)

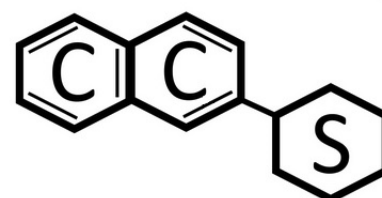
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face 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 protection

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).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

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).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 240 min

Material tested: Camatril® (KCL 730 / Size M)

Body Protection

protective clothing

Respiratory protection

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

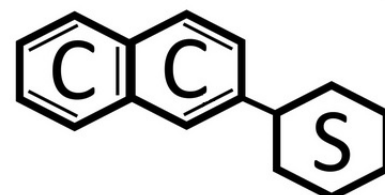
The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

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.

Control of environmental exposure

Do not let product enter drains.



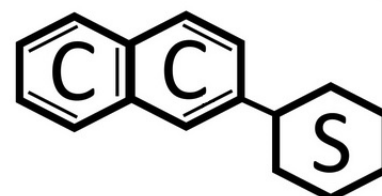
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Color: colorless
b) Odor	unpleasant
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/cm ³ 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

Forms explosive mixtures with air on intense heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:
alkalines
Amines
Nitriles
Oxidizing agents

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

No data available

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.

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)

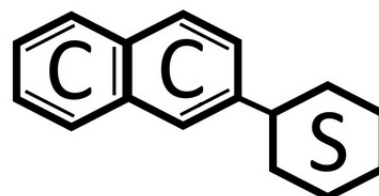
Serious eye damage/eye irritation

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 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

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: (ECHA)

The value is given in analogy to the following substances: Sodium isovalerate-1-13C

RTECS: NY1400000

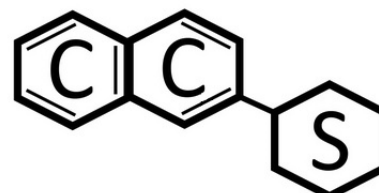
Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Inhalation may provoke the following symptoms:, spasm, inflammation and edema of the bronchi, spasm, inflammation and edema of the larynx, pneumonitis, pulmonary edema, Symptoms and signs 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: 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: 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: 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) Remarks: The value is given in analogy to the following substances: valeric acid
Toxicity to bacteria	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

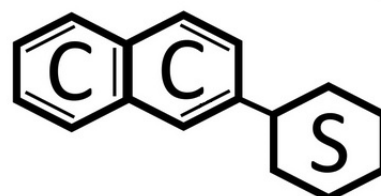
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

Discharge into the environment must be avoided.



SECTION 13: Disposal considerations**13.1 Waste treatment methods****Product**

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**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
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

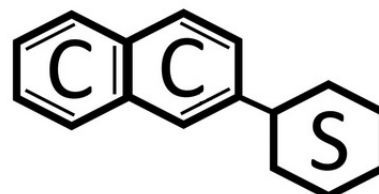
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

3-methylbutyric acid	CAS-No. 503-74-2	Revision Date 1993-04-24
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SECTION 16: Other information**Further information**

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Consolidated Chemicals LLC and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product.

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