

Chemical Safety Data Sheet MSDS / SDS

Isovaleric acid

Revision Date:2024-07-06 Revision Number:1

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

Product identifier

Product name : Isovaleric acid
CBnumber : CB8729604
CAS : 503-74-2
EINECS Number : 207-975-3
Synonyms : ISOVALERIC ACID,3-methylbutanoic acid

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P405 Store locked up.

P310 Immediately call a POISON CENTER or doctor/physician.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

Hazard statements

H318 Causes serious eye damage

H314 Causes severe skin burns and eye damage

H227 Combustible liquid

SECTION 3: Composition/information on ingredients

Substance

Product name	: Isovaleric acid
Synonyms	: ISOVALERIC ACID,3-methylbutanoic acid
CAS	: 503-74-2
EC number	: 207-975-3
MF	: C5H10O2
MW	: 102.13

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

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.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

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

Unsuitable extinguishing media

Do NOT use water jet.

Special hazards arising from the substance or mixture

Carbon oxides Combustible.

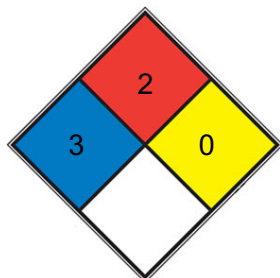
Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

Use water spray to cool unopened containers.

NFPA 704



HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

FIRE 2 Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N₂](#))

SPEC.

HAZ.

SECTION 6: Accidental release measures

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 vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

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.

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.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid inhalation of vapor or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

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. Store in cool place.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

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.

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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

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

Information on basic physicochemical properties

Appearance	colorless liquid
Odour	unpleasant
Odour Threshold	No data available
pH	3,1 at 10 g/l at 25 °C - DIN 19268
Melting point/freezing point	Melting point: ca.-31 °C - OECD Test Guideline 102
Initial boiling point and boiling range	178,5 °C at 1.013 hPa - OECD Test Guideline 103
Flash point	80 °C - Pensky-Martens closed cup - ISO 2719
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 6,8 %(V) Lower explosion limit: 1,5 %(V)
Vapour pressure	ca.1 hPa at 20 °C
Vapour density	No data available
Relative density	0,93 g/cm ³ at 20 °C
Water solubility	48 g/l at 20 °C - OECD Test Guideline 105 - completely soluble
Partition coefficient: n-octanol/water	Pow: 50; log Pow: 1,7 at 25 °C - Bioaccumulation is not expected.
Autoignition temperature	420 °C at 988 hPa - Tested according to Directive 92/69/EEC.
Decomposition temperature	>300 °C -
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

Surface tension 63,3 mN/m at 1g/l at 20 °C

OECD Test Guideline 115

Dissociation constant 4,7 at 20,1 °C

OECD Test Guideline 112

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

Heat, flames and sparks.

Incompatible materials

Bases, Oxidizing agents, Reducing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides Other decomposition products - No data available

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 2.500 mg/kg (OECD Test Guideline 401)

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.

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

OECD Test Guideline 474

Mouse - male and female - Red blood cells (erythrocytes)

Result: negative

(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.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Acute oral toxicity - If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

Acute inhalation toxicity - mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

Repeated dose toxicity - Rat - male - Oral - 90 Days - NOAEL (No observed adverse effect level) - 5.000 mg/kg

(in analogy to similar products) (ECHA) 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.

Toxicity

LD50 i.v. in mice: 1120±30 mg/kg (Or, Wretlind)

SECTION 12: Ecological information

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)

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)

Toxicity to algae

static test ErC50 - Pseudokirchneriella subcapitata - 29,3 mg/l - 72 h (OECD Test Guideline 201)

Remarks: (in analogy to similar products)

static test NOEC - Pseudokirchneriella subcapitata - 6,38 mg/l - 72 h (OECD Test Guideline 201)

Remarks: (in analogy to similar products)

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)

Persistence and degradability

Biodegradability aerobic - Exposure time 10 d

Result: 58 - 66 % - Readily biodegradable. (OECD Test Guideline 301C)

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

Harmful to aquatic life.

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 3265 IMDG: 3265 IATA: 3265

UN proper shipping name

ADR/RID: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (3-methylbutyric acid) IMDG: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (3-methylbutyric acid)

IATA: Corrosive liquid, acidic, organic, n.o.s. (3-methylbutyric acid)

Transport hazard class(es)

ADR/RID: 8 IMDG: 8 IATA: 8

Packaging group

ADR/RID: II IMDG: II IATA: II

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

EC Inventory:Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

References

[1] CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

[2] ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

[3] ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

[4] eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

[5] ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
Chemical Book

【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Disclaimer:

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