

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isovaleric acid > 99 % for gas chromatography

Revision date: 22.09.2023

Product code: 27588

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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**

Isovaleric acid > 99 % for gas chromatography

CAS No: 503-74-2

EC No: 207-975-3

1.2. Relevant identified uses of the substance or mixture and uses advised against**Use of the substance/mixture**

Laboratory chemical

Industrial uses: Uses of substances as such or in preparations at industrial sites

Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Uses advised against

Do not use for private purposes (household).

1.3. Details of the supplier of the safety data sheet

Company name: AnalytiChem GmbH

Street: Stempelstraße 6

Place: D-47167 Duisburg

Telephone: 0203/5194-0

Telefax: 0203/5194-290

E-mail: info@analytichem.de

Contact person: Abteilung Produktsicherheit

Telephone: 0203/5194-107/117

E-mail: produktsicherheit@analytichem.de

Internet: www.analytichem.de

Responsible Department: Abteilung Produktsicherheit

1.4. Emergency telephone number:

For Hazardous Materials [or Dangerous Goods] Incidents Spill, Leak, Fire, Exposure, or Accident Call CHEMTREC Day or Night Within USA and Canada: 1-800-424-9300 Outside USA and Canada: +1 703-741-5970 (collect calls accepted)

Further Information

A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

SECTION 2: Hazards identification**2.1. Classification of the substance or mixture****Regulation (EC) No 1272/2008**

Met. Corr. 1; H290

Skin Corr. 1B; H314

Full text of hazard statements: see SECTION 16.

2.2. Label elements**Regulation (EC) No 1272/2008**

Signal word: Danger

Pictograms:

**Hazard statements**

H290

May be corrosive to metals.

H314

Causes severe skin burns and eye damage.

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Precautionary statements

P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P301+P330+P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308	IF exposed or concerned:
P310	Immediately call a POISON CENTER/doctor.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula:	C ₅ H ₁₀ O ₂
Molecular weight:	102,13 g/mol

Hazardous components

CAS No	Chemical name	Quantity
	EC No	Index No
		REACH No
	Classification (Regulation (EC) No 1272/2008)	
503-74-2	isovaleric acid	100 %
	207-975-3	
	Met. Corr. 1, Skin Corr. 1B; H290 H314	

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
503-74-2	207-975-3	isovaleric acid	100 %
	dermal: LD50 = > 2000 mg/kg; oral: LD50 = ca. 2500 mg/kg		

Further Information

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of = 0.1 % (w/w).

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

Self-protection of the first aider

After inhalation

Provide fresh air.
Call a physician immediately.

After contact with skin

Wash immediately with: Water, Polyethylene glycol 400
Take off immediately all contaminated clothing and wash it before reuse.
Call a physician immediately.

After contact with eyes

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.
Remove contact lenses, if present and easy to do. Continue rinsing.

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After ingestion

- Rinse mouth immediately and drink plenty of water.
- Do NOT induce vomiting.
- Do not allow a neutralisation agent to be drunk.
- Call a physician immediately.

4.2. Most important symptoms and effects, both acute and delayed

- Gastrointestinal complaints
- Cough, Dyspnoea
- Irritant, corrosive
- Risk of serious damage to eyes.

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
- Extinguishing powder

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

- Combustible liquids
- Hazardous combustion products
- In case of warming:
Vapours are heavier than air, spread along floors and form explosive mixtures with air.

5.3. Advice for firefighters

- Wear a self-contained breathing apparatus and chemical protective clothing.
- Avoid contact with skin, eyes and clothes.

Additional information

- Suppress gases/vapours/mists with water spray jet.
- Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General advice

Corrosive to metals.

For non-emergency personnel

- Provide adequate ventilation.
- Use personal protection equipment.
- Avoid contact with skin, eyes and clothes.
- Remove persons to safety.
- Emergency procedures
- Do not breathe dust/fume/gas/mist/vapours/spray.

For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up

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For containment

- Cover drains.
- Prevent spread over a wide area (e.g. by containment or oil barriers).
- Collect in closed and suitable containers for disposal.
- Take up carefully when dry. Take up dust-free and set down dust-free.

For cleaning up

- Clean contaminated articles and floor according to the environmental legislation.

Other information

- Provide adequate ventilation.
- Do not breathe dust/fume/gas/mist/vapours/spray.
- Wear breathing apparatus if exposed to vapours/dusts/aerosols.

6.4. Reference to other sections

- Safe handling: see section 7
- Personal protection equipment: see section 8
- Disposal: see section 13

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

- Do not breathe vapour/aerosol.
- Read label before use.

Advice on protection against fire and explosion

- Usual measures for fire prevention.

Advice on general occupational hygiene

- Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme.
- Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat or drink.

Further information on handling

- Draw up and observe skin protection programme.
- Wash hands and face before breaks and after work and take a shower if necessary.
- Take off immediately all contaminated clothing and wash it before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

- Keep container tightly closed.
- Store in a dry place.

Further information on storage conditions

- Keep cool. Protect from sunlight.
- storage temperature +15°C - +25°C.

7.3. Specific end use(s)

- Laboratory chemicals

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

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PNEC values

CAS No	Substance	
Environmental compartment		Value
503-74-2	isovaleric acid	
Freshwater		0,0293 mg/l
Freshwater (intermittent releases)		0,293 mg/l
Marine water		0,00293 mg/l
Freshwater sediment		0,1173 mg/kg
Marine sediment		0,0117 mg/kg
Micro-organisms in sewage treatment plants (STP)		22,4 mg/l
Soil		0,00625 mg/kg

8.2. Exposure controls

Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection equipment.

Provide adequate ventilation as well as local exhaust at critical locations.

Individual protection measures, such as personal protective equipment

Eye/face protection

Suitable eye protection: goggles.

Hand protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: vertrieb@kcl.de With specification (test according to EN374):

By long-term hand contact

Trade name/designation: KCL 898 Butoject®

Recommended material: Butyl caoutchouc (butyl rubber) 0,7 mm

Wearing time with permanent contact: > 480 min

By short-term hand contact

Trade name/designation: KCL 730 Camatril® Velours

Recommended material: NBR (Nitrile rubber) 0,4 mm

Wearing time with occasional contact (splashes): > 240 min

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types. 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Skin protection

Wear suitable protective clothing.

Respiratory protection

Respiratory protection necessary at: aerosol or mist formation

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Environmental exposure controls

Do not allow to enter into surface water or drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	Liquid
Colour:	colourless
Odour:	characteristic rancid
Odour threshold:	No data available
Melting point/freezing point:	-26 °C
Boiling point or initial boiling point and boiling range:	176 °C
Flammability:	No data available
Lower explosion limits:	1,5 vol. %
Upper explosion limits:	6,8 vol. %
Flash point:	74 °C
Auto-ignition temperature:	440 °C
Decomposition temperature:	No data available
pH-Value (at 20 °C):	20 (10 g/l)
Viscosity / kinematic:	No data available
Water solubility: (at 20 °C)	25 g/L
Solubility in other solvents	No data available
Dissolution rate:	No data available
Partition coefficient n-octanol/water:	No data available
Dispersion stability:	No data available
Vapour pressure: (at 20 °C)	0,5 hPa
Vapour pressure: (at 50 °C)	3,7 hPa
Density (at 20 °C):	0,93 g/cm ³
Relative density:	No data available
Bulk density:	No data available
Relative vapour density:	No data available
Particle characteristics:	No data available

9.2. Other information

Information with regard to physical hazard classes

Sustaining combustion:	No data available
Self-ignition temperature	
Solid:	No data available
Gas:	No data available
Oxidizing properties	
Not oxidising.	

Other safety characteristics

Evaporation rate:	No data available
Solvent separation test:	No data available
Solvent content:	No data available
Solid content:	No data available
Sublimation point:	No data available
Softening point:	No data available
Pour point:	No data available

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No data available:

Viscosity / dynamic:
(at 20 °C)

2,4 mPa·s

Flow time:

No data available

Further Information

Corrosive to metals.

SECTION 10: Stability and reactivity

10.1. Reactivity

In case of warming:

Vapours are heavier than air, spread along floors and form explosive mixtures with air.

10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

10.3. Possibility of hazardous reactions

Violent reaction with:

Oxidising agent

Amines

Nitriles

alkalines

10.4. Conditions to avoid

Heat

10.5. Incompatible materials

Metal

10.6. Hazardous decomposition products

No data available

Further information

No data available

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Toxicokinetics, metabolism and distribution

No data available

Acute toxicity

Based on available data, the classification criteria are not met.

If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects).

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
503-74-2	isovaleric acid				
	oral	LD50 mg/kg ca. 2500	Rat	Study report (1980)	OECD Guideline 401
	dermal	LD50 mg/kg > 2000	Rabbit	Study report (1990)	OECD Guideline 402

Irritation and corrosivity

Causes severe skin burns and eye damage.

Causes serious eye damage.

Risk of serious damage to eyes.

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Sensitising effects

Based on available data, the classification criteria are not met.

Carcinogenic/mutagenic/toxic effects for reproduction

Based on available data, the classification criteria are not met.

STOT-single exposure

Based on available data, the classification criteria are not met.

STOT-repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

Based on available data, the classification criteria are not met.

Information on likely routes of exposure

No data available

Specific effects in experiment on an animal

No data available

Additional information on tests

No data available

Practical experience

No data available

11.2. Information on other hazards

Endocrine disrupting properties

No data available

Other information

No data available

Further information

Gastrointestinal complaints

Cough, Dyspnoea

Irritant, corrosive

Risk of serious damage to eyes.

SECTION 12: Ecological information

12.1. Toxicity

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
503-74-2	isovaleric acid					
	Acute fish toxicity	LC50 77 mg/l	96 h	Pimephales promelas	Publication (1976)	OECD Guideline 203
	Acute algae toxicity	ErC50 mg/l 45,1	72 h	Desmodesmus subspicatus	Study report (1990)	other: German industrial standard test g
	Acute crustacea toxicity	EC50 mg/l 51,25	48 h	Daphnia magna	Study report (1989)	other: German industrial standard test g

12.2. Persistence and degradability

>65%

12.3. Bioaccumulative potential

No data available

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Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
503-74-2	isovaleric acid	50

BCF

CAS No	Chemical name	BCF	Species	Source
503-74-2	isovaleric acid	3,162		Other company data (

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

12.7. Other adverse effects

Discharge into the environment must be avoided.

Further information

Do not allow to enter into surface water or drains.

SECTION 13: Disposal considerations**13.1. Waste treatment methods****Disposal recommendations**

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.

Do not mix with other wastes.

Do not empty into drains.

Send to a physico-chemical treatment facility under observation of official regulations.

Contaminated packaging

Handle contaminated packages in the same way as the substance itself.

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

SECTION 14: Transport information**Land transport (ADR/RID)**

14.1. UN number or ID number:	UN 3265
14.2. UN proper shipping name:	CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (isovaleric acid)
14.3. Transport hazard class(es):	8
14.4. Packing group:	II
Hazard label:	8
Classification code:	C3
Special Provisions:	274
Limited quantity:	1 L
Excepted quantity:	E2
Transport category:	2
Hazard No:	80
Tunnel restriction code:	E

Inland waterways transport (ADN)

14.1. UN number or ID number:	UN 3265
14.2. UN proper shipping name:	CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (isovaleric acid)
14.3. Transport hazard class(es):	8
14.4. Packing group:	II
Hazard label:	8

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Classification code: C3
Special Provisions: 274
Limited quantity: 1 L
Excepted quantity: E2

Marine transport (IMDG)

14.1. UN number or ID number: UN 3265
14.2. UN proper shipping name: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (isovaleric acid)
14.3. Transport hazard class(es): 8
14.4. Packing group: II
Hazard label: 8
Special Provisions: 274
Limited quantity: 1 L
Excepted quantity: E2
EmS: F-A, S-B

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number: UN 3265
14.2. UN proper shipping name: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (isovaleric acid)
14.3. Transport hazard class(es): 8
14.4. Packing group: II
Hazard label: 8
Special Provisions: A3 A803
Limited quantity Passenger: 0.5 L
Passenger LQ: Y840
Excepted quantity: E2
IATA-packing instructions - Passenger: 851
IATA-max. quantity - Passenger: 1 L
IATA-packing instructions - Cargo: 855
IATA-max. quantity - Cargo: 30 L

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

No dangerous good in sense of this transport regulation.

14.7. Maritime transport in bulk according to IMO instruments

not applicable

SECTION 15: Regulatory information

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

EU regulatory information

Restrictions on use (REACH, annex XVII):

Entry 3

Information according to 2012/18/EU (SEVESO III): Not subject to 2012/18/EU (SEVESO III)

National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

Water hazard class (D): 1 - slightly hazardous to water

SECTION 16: Other information

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Changes

This data sheet contains changes from the previous version in section(s): 12.

Abbreviations and acronyms

ADR: Accord européen sur le transport des marchandises dangereuses par Route
(European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service

LC50: Lethal concentration, 50%

LD50: Lethal dose, 50%

Met. Corr: Substance or mixture corrosive to metals

Skin Corr: Skin corrosion

Eye Dam: Eye damage

Relevant H and EUH statements (number and full text)

H290 May be corrosive to metals.

H314 Causes severe skin burns and eye damage.

H318 Causes serious eye damage.

Further Information

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material. The receiver of our product is singularly responsible for adhering to existing laws and regulations.