

Safety Data Sheet

according to Regulation (EC) No 1907/2006

iso-Butyric acid > 99 % for gas chromatography

Revision date: 13.07.2023

Product code: 27586

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

1.1. Product identifier

iso-Butyric acid > 99 % for gas chromatography

CAS No: 79-31-2
Index No: 607-063-00-9
EC No: 201-195-7

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

Use of the substance/mixture

Laboratory chemicals

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
E-mail: info@analytichem.de
Contact person: Abteilung Produktsicherheit
E-mail: produktsicherheit@analytichem.de
Internet: www.analytichem.de
Responsible Department: Abteilung Produktsicherheit

Telefax: 0203/5194-290

Telephone: 0203/5194-107/117

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

Flam. Liq. 3; H226
Acute Tox. 3; H311
Acute Tox. 4; H302
Skin Corr. 1B; H314
Eye Dam. 1; H318

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Danger

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Pictograms:



Hazard statements

H226	Flammable liquid and vapour.
H302	Harmful if swallowed.
H311	Toxic in contact with skin.
H314	Causes severe skin burns and eye damage.

Precautionary statements

P260	Do not breathe dust/fume/gas/mist/vapours/spray.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P303+P361+P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
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:	(CH ₃) ₂ CHCOOH
Molecular weight:	88,11 g/mol

Hazardous components

CAS No	Chemical name	Quantity
	EC No	Index No
		REACH No
	Classification (Regulation (EC) No 1272/2008)	
79-31-2	isobutyric acid	100 %
	201-195-7	607-063-00-9
	Flam. Liq. 3, Acute Tox. 3, Acute Tox. 4, Skin Corr. 1B, Eye Dam. 1; H226 H311 H302 H314 H318	

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		
79-31-2	201-195-7	isobutyric acid	100 %
	dermal: ATE = 300 mg/kg; oral: LD50 = 2230 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

No data available

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After inhalation

Provide fresh air.
Call a doctor if you feel unwell.

After contact with skin

Wash immediately with: Water
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.

After ingestion

Rinse mouth immediately and drink plenty of water.
Call a physician immediately.

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

Irritant
corrosive
Cough
Dyspnoea
Vapours may cause drowsiness and dizziness.
Vomiting
Headache

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 fire may be liberated: Carbon dioxide (CO₂) Carbon monoxide
In case of warming:
Vapours are heavier than air, spread along floors and form explosive mixtures with air.
Heating causes rise in pressure with risk of bursting.
Beware of reignition.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.
In case of fire and/or explosion do not breathe fumes.
Avoid contact with skin, eyes and clothes.

Additional information

Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.
Move undamaged containers from immediate hazard area if it can be done safely.
Use water spray jet to protect personnel and to cool endangered containers.

SECTION 6: Accidental release measures

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6.1. Personal precautions, protective equipment and emergency procedures

General advice

Keep away from sources of ignition - No smoking.

This material can be ignited by heat, sparks, flames, or other sources of ignition (e.g., static electricity, pilot lights, mechanical/electrical equipment, and electronic devices such as cell phones, computers, calculators, and pagers which have not been certified as intrinsically safe).

Take action to prevent static discharges.

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.

The vapour of the product is heavier than air and may accumulate below ground level, in pits, channels and basements in higher concentration.

Danger of explosion

6.3. Methods and material for containment and cleaning up

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.

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

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

Read label before use. Handle and open container with care.

When using do not eat, drink, smoke, sniff. Keep container tightly closed.

Use personal protection equipment. Use extractor hood (laboratory).

Do not breathe vapour/aerosol. Provide adequate ventilation.

Advice on protection against fire and explosion

Take action to prevent static discharges. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

Wash hands and face before breaks and after work and take a shower if necessary.

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When using do not eat or drink.

Avoid: aerosol or mist formation Do not breathe vapour/aerosol.

Further information on handling

Take off immediately all contaminated clothing and wash it before reuse.

Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary. If handled uncovered, arrangements with local exhaust ventilation have to be used.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container tightly closed in a cool, well-ventilated place.

Store in a cool dry place.

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Further information on storage conditions

Protect from sunlight.

storage temperature +15°C - +25°C

Store in a place accessible by authorized persons only.

7.3. Specific end use(s)

Laboratory chemicals

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

DNEL/DMEL values

CAS No	Substance	Exposure route	Effect	Value
79-31-2	isobutyric acid			
Worker DNEL, long-term		inhalation	systemic	184 mg/m ³
Worker DNEL, long-term		dermal	systemic	3,75 mg/kg bw/day
Consumer DNEL, long-term		inhalation	systemic	92 mg/m ³
Consumer DNEL, long-term		dermal	systemic	1,88 mg/kg bw/day
Consumer DNEL, long-term		oral	systemic	1,88 mg/kg bw/day

PNEC values

CAS No	Substance	Value
79-31-2	isobutyric acid	
Freshwater		0,045 mg/l
Freshwater (intermittent releases)		0,451 mg/l
Marine water		0,004 mg/l
Freshwater sediment		0,364 mg/kg
Marine sediment		0,036 mg/kg
Micro-organisms in sewage treatment plants (STP)		19 mg/l
Soil		0,046 mg/kg

8.2. Exposure controls

Appropriate engineering controls

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

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equipment.

If handled uncovered, arrangements with local exhaust ventilation have to be used.

Individual protection measures, such as personal protective equipment

Eye/face protection

goggles

Face protection umbrella

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 897 Butoject®

Suitable material: Butyl caoutchouc (butyl rubber) 0,3 mm

Wearing time with permanent contact: > 480 min

By short-term hand contact

Trade name/designation KCL 730 Camatril® Velours

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

Wearing time with occasional contact (splashes): > 60 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 fire resistant or flame retardant clothing.

Take off immediately all contaminated clothing and wash it before reuse.

Wear suitable protective clothing. Take off immediately all contaminated clothing.

Wash hands and face before breaks and after work and take a shower if necessary.

Respiratory protection

Wear breathing apparatus if exposed to vapours/dusts/aerosols.

Filtering device with filter or ventilator filtering device of type: A

Environmental exposure controls

Do not allow to enter into surface water or drains.

Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches.

Danger of explosion

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	Liquid	
Colour:	colourless	
Odour:	stinging	
Odour threshold:	No data available	
Melting point/freezing point:		-45 °C
Boiling point or initial boiling point and boiling range:		156 °C

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Flammability:	No data available
Lower explosion limits:	2 vol. %
Upper explosion limits:	12 vol. %
Flash point:	57,5 °C
Auto-ignition temperature:	420 °C
Decomposition temperature:	No data available
pH-Value:	No data available
Viscosity / kinematic:	No data available
Water solubility: (at 20 °C)	210 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)	12 hPa
Vapour pressure:	No data available
Density:	0,95 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

Explosive properties

In case of warming:

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

Sustaining combustion:

Sustaining combustion

Self-ignition temperature

Solid:

No data available

Gas:

No data available

Oxidizing properties

No data available

Other safety characteristics

Evaporation rate:

No data available

Solvent separation test:

No data available

Solvent content:

100%

Solid content:

No data available

Sublimation point:

No data available

Softening point:

No data available

Pour point:

No data available

Viscosity / dynamic:

1,12 mPa·s

(at 20 °C)

Flow time:

No data available

Further Information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

In case of warming:

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Vapours may 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

Oxidising agent
Reducing agent
metals
Amines
Nitriles
Alkali (lye)
Isocyanates

10.4. Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

10.5. Incompatible materials

Aluminium
Zinc
metals

10.6. Hazardous decomposition products

SECTION 5: Firefighting measures

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

Toxic in contact with skin.
Harmful if swallowed.

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
79-31-2	isobutyric acid				
	oral	LD50 mg/kg	2230	Rat	Study report (1985) OECD Guideline 401
	dermal	ATE mg/kg	300		

Irritation and corrosivity

Causes severe skin burns and eye damage.
Causes serious eye damage.

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.

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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

This product does not contain a substance that has endocrine disrupting properties with respect to humans as no components meets the criteria.

Other information

Pulmonary oedema

Pneumonia

Further information

Irritant

corrosive

Cough

Dyspnoea

Vapours may cause drowsiness and dizziness.

Vomiting

Headache

SECTION 12: Ecological information

12.1. Toxicity

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

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
79-31-2	isobutyric acid					
	Acute fish toxicity	LC50 mg/l	146,6	96 h	Leuciscus idus	REACH Registration Dossier other: German industrial standard test g
	Acute algae toxicity	ErC50 mg/l	45,1	72 h	Desmodesmus subspicatus	REACH Registration Dossier other: German industrial standard test g
	Acute crustacea toxicity	EC50 mg/l	51,25	48 h	Daphnia magna	REACH Registration Dossier other: German industrial standard test g

12.2. Persistence and degradability

100 %

Readily biodegradable (according to OECD criteria).

12.3. Bioaccumulative potential

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
79-31-2	isobutyric acid	12,6

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BCF

CAS No	Chemical name	BCF	Species	Source
79-31-2	isobutyric acid	3,16		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

Avoid release to the environment.

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.

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

Do not empty into drains.

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 2529
14.2. UN proper shipping name:	ISOBUTYRIC ACID
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3+8
Classification code:	FC
Limited quantity:	5 L
Excepted quantity:	E1
Transport category:	3
Hazard No:	38
Tunnel restriction code:	D/E

Inland waterways transport (ADN)

14.1. UN number or ID number:	UN 2529
14.2. UN proper shipping name:	ISOBUTYRIC ACID
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3+8
Classification code:	FC
Limited quantity:	5 L
Excepted quantity:	E1

Marine transport (IMDG)

14.1. UN number or ID number:	UN 2529
14.2. UN proper shipping name:	ISOBUTYRIC ACID

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14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3+8
Special Provisions:	-
Limited quantity:	5 L
Excepted quantity:	E1
EmS:	F-E, S-C

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number:	UN 2529
14.2. UN proper shipping name:	ISOBUTYRIC ACID
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3+8
Special Provisions:	A803
Limited quantity Passenger:	1 L
Passenger LQ:	Y342
Excepted quantity:	E1
IATA-packing instructions - Passenger:	354
IATA-max. quantity - Passenger:	5 L
IATA-packing instructions - Cargo:	365
IATA-max. quantity - Cargo:	60 L

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, Entry 40

Information according to 2012/18/EU (SEVESO III): P5c FLAMMABLE LIQUIDS

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

Changes

This data sheet contains changes from the previous version in section(s): 11,12.

Abbreviations and acronyms

Flam. Liq: Flammable liquid

Acute Tox: Acute toxicity

Skin Corr: Skin corrosion

Eye Dam: Eye damage

Relevant H and EUH statements (number and full text)

H226	Flammable liquid and vapour.
H302	Harmful if swallowed.
H311	Toxic in contact with skin.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.

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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 information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights.

The receiver of our product is singularly responsible for adhering to existing laws and regulations.