

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYRIC ACID

Revision date: 21.09.2022

Product code: 222200

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

1.1. Product identifier

NATURAL ISOBUTYRIC ACID

Substance name:	NATURAL ISOBUTYRIC ACID
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

For Flavour use for food and feed only

1.3. Details of the supplier of the safety data sheet

Company name:	Axxence Aromatic GmbH	
Street:	Tackenweide 28	
Place:	D-46446 Emmerich am Rhein	
Telephone:	+ 49 2822 68561 0	Telefax: + 49 2822 68561 39
E-mail:	info@axxence.com	
Contact person:	Safety Team	Telephone: + 49 2822 68561 0
E-mail:	safety-documentation@axxence.com	
Internet:	www.axxence.de	
Responsible Department:	Safety Management	

1.4. Emergency telephone number:

+49 2822 68561 99

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. 1; H314

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Danger

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

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.

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P240	Ground and bond container and receiving equipment.
P241	Use explosion-proof electrical/ventilating/lighting equipment.
P242	Use non-sparking tools.
P243	Take action to prevent static discharges.
P260	Do not breathe dust/fume/gas/mist/vapours/spray.
P264	Wash hands thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P301+P330+P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P312	Call a POISON CENTER/doctor if you feel unwell.
P302+P352	IF ON SKIN: Wash with plenty of Water and soap.
P303+P361+P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P312	Call a POISON CENTER/doctor if you feel unwell.
P361+P364	Take off immediately all contaminated clothing and wash it before reuse.
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P310	Immediately call a POISON CENTER/doctor.
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.
P403+P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/container to organic waste.

2.3. Other hazards

No information available.

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula:	C4 H8 O2
Molecular weight:	88,11 g/mol

Relevant ingredients

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
79-31-2	NATURAL ISOBUTYRIC ACID			100 %
	201-195-7	607-063-00-9		
	Flam. Liq. 3, Acute Tox. 3, Acute Tox. 4, Skin Corr. 1; H226 H311 H302 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	
79-31-2	201-195-7	NATURAL ISOBUTYRIC ACID	100 %
		dermal: LD50 = 475 mg/kg; oral: LD50 = < 2000 mg/kg	

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

First aider: Pay attention to self-protection! Remove affected person from the danger area and lay down.

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After inhalation

Provide fresh air. Medical treatment necessary.

After contact with skin

After contact with skin, wash immediately with plenty of water and soap. 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.

After ingestion

Rinse mouth immediately and drink 1 glass of water. Do NOT induce vomiting. Adverse human health effects and symptoms: Gastric perforation. Call a physician immediately. Do not allow a neutralisation agent to be drunk.

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

No information available.

4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5: Firefighting measures**5.1. Extinguishing media****Suitable extinguishing media**

Water spray jet, Carbon dioxide (CO₂), Foam, Extinguishing powder.

5.2. Special hazards arising from the substance or mixture

Flammable. Vapours can form explosive mixtures with air.

5.3. Advice for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing. Full protection suit.

Additional information

Use water spray jet to protect personnel and to cool endangered containers. 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**

Remove all sources of ignition. Do not breathe gas/fumes/vapour/spray. Avoid contact with skin, eyes and clothes. Use personal protection equipment.

6.2. Environmental precautions

Do not allow uncontrolled discharge of product into the environment. Explosion risk.

6.3. Methods and material for containment and cleaning up**For cleaning up**

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents). Treat the recovered material as prescribed in the section on waste disposal.

Other information

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents). Treat the recovered material as prescribed in the section on waste disposal.

6.4. Reference to other sections

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13

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SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe gas/fumes/vapour/spray.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges. Vapours can form explosive mixtures with air.

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, drink, smoke, sniff. 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, drink, smoke, sniff.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container tightly closed. Keep locked up. Store in a place accessible by authorized persons only. Provide adequate ventilation as well as local exhaustion at critical locations. Keep in a cool, well-ventilated place. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Hints on joint storage

Do not store together with: Oxidizing agent. Pyrophoric or self-heating substances.

7.3. Specific end use(s)

For Flavour use for food and feed only

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

DNEL/DMEL values

CAS No	Name of agent	Exposure route	Effect	Value
79-31-2	NATURAL 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
Consumer DNEL, acute		oral	systemic	2230 mg/kg bw/day
Consumer DNEL, acute		inhalation	systemic	9590 mg/m ³
Consumer DNEL, acute		dermal	systemic	474 mg/kg bw/day

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PNEC values

CAS No	Name of agent	
Environmental compartment		Value
79-31-2	NATURAL ISOBUTYRIC ACID	
Freshwater		0,045 mg/l
Freshwater (intermittent releases)		0,45 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

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe gas/fumes/vapour/spray.

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. Suitable gloves type: NBR (Nitrile rubber) + Natural fibres (e.g. cotton)

Skin protection

Use of protective clothing.

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	Liquid
Colour:	
Odour:	stinging
Melting point/freezing point:	-64 °C
Boiling point or initial boiling point and boiling range:	156 °C
Flammability:	not applicable not applicable
Lower explosion limits:	not determined
Upper explosion limits:	not determined
Flash point:	58 °C
Auto-ignition temperature:	455 °C
Decomposition temperature:	not determined

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pH-Value (at 20 °C):	2,3
Viscosity / kinematic: (at 20 °C)	1,39 mm ² /s
Water solubility: (at 20 °C)	618 g/l
Solubility in other solvents not determined	
Partition coefficient n-octanol/water:	1,1
Vapour pressure: (at 20 °C)	1,81 hPa
Vapour pressure: (at 50 °C)	12,5 hPa
Density (at 20 °C):	0,95 g/cm ³
Relative vapour density: (at 20 °C)	3,04

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

not explosive according to EU A.14

Oxidizing properties

The product is not: oxidising.

Other safety characteristics

Evaporation rate: not determined

Solvent content: 0%

Solid content: 0%

Viscosity / dynamic:
(at 20 °C) 1,32 mPa·s

SECTION 10: Stability and reactivity

10.1. Reactivity

Flammable.

10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

10.3. Possibility of hazardous reactions

No known hazardous reactions.

10.4. Conditions to avoid

Keep away from sources of heat (e.g. hot surfaces), sparks and open flames. Vapours can form explosive mixtures with air.

10.5. Incompatible materials

No information available.

10.6. Hazardous decomposition products

No known hazardous decomposition products.

SECTION 11: Toxicological information

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

Acute toxicity

Toxic in contact with skin.

Harmful if swallowed.

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CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
79-31-2	NATURAL ISOBUTYRIC ACID				
	oral	LD50 mg/kg	< 2000	Rat	Gestis
	dermal	LD50 mg/kg	475	Rabbit	Gestis

Irritation and corrosivity

Skin corrosion/irritation: Causes severe skin burns and eye damage.

Serious eye damage/eye irritation: Causes serious eye damage.

Sensitising effects

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

Carcinogenic/mutagenic/toxic effects for reproduction

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

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

Reproductive toxicity: 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.

11.2. Information on other hazards

Endocrine disrupting properties

No information available.

SECTION 12: Ecological information

12.1. Toxicity

The product is not: Ecotoxic.

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
79-31-2	NATURAL ISOBUTYRIC ACID					
	Acute fish toxicity	LC50	147 mg/l	96 h	Leuciscus idus (golden orfe)	REACH reg. OECD TG 203

12.2. Persistence and degradability

The product has not been tested.

CAS No	Chemical name			
	Method	Value	d	Source
	Evaluation			
79-31-2	NATURAL ISOBUTYRIC ACID			
	similar to OECD TG 302 B	>95%	10	
	Readily biodegradable			

12.3. Bioaccumulative potential

The product has not been tested.

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Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
79-31-2	NATURAL ISOBUTYRIC ACID	1,1

BCF

CAS No	Chemical name	BCF	Species	Source
79-31-2	NATURAL ISOBUTYRIC ACID	3,16		

12.4. Mobility in soil

The product has not been tested.

12.5. Results of PBT and vPvB assessment

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

The product has not been tested.

12.6. Endocrine disrupting properties

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

12.7. Other adverse effects

No information available.

Further information

Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal recommendations

Do not allow to enter into surface water or drains. Dispose of waste according to applicable legislation.

List of Wastes Code - residues/unused products

160305 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; off-specification batches and unused products; organic wastes containing hazardous substances; hazardous waste

List of Wastes Code - used product

160305 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; off-specification batches and unused products; organic wastes containing hazardous substances; hazardous waste

List of Wastes Code - contaminated packaging

150110 WASTE PACKAGING; ABSORBENTS, WIPING CLOTHS, FILTER MATERIALS AND PROTECTIVE CLOTHING NOT OTHERWISE SPECIFIED; packaging (including separately collected municipal packaging waste); packaging containing residues of or contaminated by hazardous substances; hazardous waste

Contaminated packaging

Hazardous waste according to Directive 2008/98/EC (waste framework directive). Handle contaminated packages in the same way as the substance itself.

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

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Limited quantity: 5 L
 Excepted quantity: E1
 Transport category: 3
 Hazard No: 38
 Tunnel restriction code: D/E

Other applicable information (land transport)

E1

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

Other applicable information (inland waterways transport)

E1

Marine transport (IMDG)

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: -
 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

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14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

Warning: Combustible liquid. strongly corrosive.

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, Entry 40

Directive 2010/75/EU on industrial emissions: 100 % (950 g/l)

Directive 2004/42/EC on VOC in paints and varnishes: 100 % (950 g/l)

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

Additional information

To follow: 850/2004/EC, 1107/2009/EC, 649/2012/EC

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

Skin resorption/Sensitization: Permeates easily through outer skin and causes poisoning.

15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

SECTION 16: Other information**Changes**

This data sheet contains changes from the previous version in section(s): 2,5,6,7,8,9,10,11,15,16.

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Abbreviations and acronyms

Flam. Liq: Flammable liquid

Acute Tox: Acute toxicity

Skin Corr: Skin corrosion

Eye Dam: Eye damage

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%

CLP: Classification, labelling and Packaging

REACH: Registration, Evaluation and Authorization of Chemicals

GHS: Globally Harmonised System of Classification, Labelling and Packaging of Chemicals

UN: United Nations

DNEL: Derived No Effect Level

DMEL: Derived Minimal Effect Level

PNEC: Predicted No Effect Concentration

ATE: Acute toxicity estimate

LL50: Lethal loading, 50%

EL50: Effect loading, 50%

EC50: Effective Concentration 50%

ErC50: Effective Concentration 50%, growth rate

NOEC: No Observed Effect Concentration

BCF: Bio-concentration factor

PBT: persistent, bioaccumulative, toxic

vPvB: very persistent, very bioaccumulative

RID: Regulations concerning the international carriage of dangerous goods by rail

ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways
(Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures)

EmS: Emergency Schedules

MFAG: Medical First Aid Guide

ICAO: International Civil Aviation Organization

MARPOL: International Convention for the Prevention of Marine Pollution from Ships

IBC: Intermediate Bulk Container

VOC: Volatile Organic Compounds

SVHC: Substance of Very High Concern

For abbreviations and acronyms, see table at <http://abbrev.esdscom.eu>

For abbreviations and acronyms, see: ECHA Guidance on information requirements and chemical safety assessment, chapter R.20 (Table of terms and abbreviations).

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.

Further Information

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.

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Identified uses

No	Short title	LCS	SU	PC	PROC	ERC	AC	TF	Specification
1	For Flavour use for food and feed only	-	-	-	-	-	-	-	Flavour

LCS: Life cycle stages

SU: Sectors of use

PC: Product categories

PROC: Process categories

ERC: Environmental release categories

AC: Article categories

TF: Technical functions