

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYRALDEHYDE

Revision date: 07.12.2022

Product code: 222000

Page 1 of 10

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

1.1. Product identifier

NATURAL ISOBUTYRALDEHYDE

CAS No: 78-84-2

EC No: 201-149-6

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

Use of the substance/mixture

Manufacturing of: - Air care products - Perfumes, fragrances - Pharmaceuticals - Cosmetics, personal care products - Flavouring Substances - Other

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:	Andreas Goertz	Telephone: + 49 2822 68561 37
e-mail:	andreas.goertz@axxence.com	
Internet:	www.axxence.de	
Responsible Department:	QM - Regulatory Affairs	

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. 2; H225

Eye Irrit. 2; H319

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Danger

Pictograms:



Hazard statements

H225 Highly flammable liquid and vapour.
H319 Causes serious eye irritation.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
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.
P264 Wash thoroughly after handling.

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYRALDEHYDE

Revision date: 07.12.2022

Product code: 222000

Page 2 of 10

<p>P280</p> <p>P303+P361+P353</p> <p>P305+P351+P338</p> <p>P337+P313</p> <p>P370+P378</p> <p>P403+P235</p> <p>P501</p>	<p>Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.</p> <p>IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.</p> <p>IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.</p> <p>If eye irritation persists: Get medical advice/attention.</p> <p>In case of fire: Use Water spray jet / Extinguishing powder / Foam / Carbon dioxide (CO₂) to extinguish.</p> <p>Store in a well-ventilated place. Keep cool.</p> <p>Dispose of contents/container to .</p>
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2.3. Other hazards

No information available.

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula: C₄ H₈ O
 Molecular weight: 72,11

Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
78-84-2	NATURAL ISOBUTYRALDEHYDE			100 %
	201-149-6			
	Flam. Liq. 2, Eye Irrit. 2; H225 H319			

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		
78-84-2	201-149-6	NATURAL ISOBUTYRALDEHYDE	100 %
	inhalation: LC50 = >23,6 mg/l (vapours); dermal: LD50 = 5670 mg/kg; oral: LD50 = 3730 mg/kg		

SECTION 4: First aid measures

4.1. Description of first aid measures

After inhalation

Provide fresh air.

After contact with skin

Wash with plenty of water. Take off contaminated clothing and wash it before reuse.

After contact with eyes

Rinse immediately carefully and thoroughly with eye-bath or water.

After ingestion

Observe risk of aspiration if vomiting occurs. Rinse mouth immediately and drink 1 glass of water.

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

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYRALDEHYDE

Revision date: 07.12.2022

Product code: 222000

Page 3 of 10

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**

Highly flammable. Vapours can form explosive mixtures with air.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.

Additional information

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

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

SECTION 7: Handling and storage**7.1. Precautions for safe handling****Advice on safe handling**

No special measures are necessary.

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

Take off contaminated clothing. Wash hands before breaks and after work. 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 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)

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYRALDEHYDE

Revision date: 07.12.2022

Product code: 222000

Page 4 of 10

Manufacturing of: - Air care products - Perfumes, fragrances - Pharmaceuticals - Cosmetics, personal care products - Flavouring Substances - Other

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

DNEL/DMEL values

CAS No	Name of agent		
DNEL type	Exposure route	Effect	Value
78-84-2	NATURAL ISOBUTYRALDEHYDE		
Worker DNEL, long-term	inhalation	local	120 mg/m ³
Consumer DNEL, acute	inhalation	local	60 mg/m ³

PNEC values

CAS No	Name of agent	
Environmental compartment	Value	
78-84-2	NATURAL ISOBUTYRALDEHYDE	
Freshwater	0,023 mg/l	
Freshwater (intermittent releases)	0,23 mg/l	
Marine water	0,0023 mg/l	
Freshwater sediment	0,086 mg/kg	
Marine sediment	0,009 mg/kg	
Micro-organisms in sewage treatment plants (STP)	10 mg/l	
Soil	0,004 mg/kg	

8.2. Exposure controls



Individual protection measures, such as personal protective equipment

Eye/face protection

Wear eye/face protection.

Hand protection

Suitable gloves type: Butyl caoutchouc (butyl rubber)

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.

Skin protection

Flame-retardant protective clothing. Wear anti-static footwear and clothing .

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

Thermal hazards

Flame-retardant protective clothing. Wear anti-static footwear and clothing

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYRALDEHYDE

Revision date: 07.12.2022

Product code: 222000

Page 5 of 10

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	Liquid	
Colour:	colourless	
Melting point/freezing point:		-65 °C
Boiling point or initial boiling point and boiling range:		64 °C
Flammability		
Solid/liquid:		not applicable
Gas:		not applicable
Lower explosion limits:		1,6 vol. %
Upper explosion limits:		11 vol. %
Flash point:		-24 °C
Auto-ignition temperature:		165 °C
Decomposition temperature:		not determined
pH-Value:		not determined
Viscosity / kinematic: (at 20 °C)		0,54 mm ² /s
Water solubility: (at 25 °C)		60 g/L
Solubility in other solvents		not determined
Partition coefficient n-octanol/water:		0,74
Vapour pressure: (at 20 °C)		184 hPa
Vapour pressure: (at 50 °C)		623 hPa
Density (at 20 °C):		0,79 g/cm ³
Relative vapour density: (at 20 °C)		2,48

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

The product is not: Explosive. The classification procedure needs not to be applied because there are no chemical groups present in the molecule which are associated with explosive properties.

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)		0,43 mPa·s

SECTION 10: Stability and reactivity

10.1. Reactivity

Highly flammable.

10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

10.3. Possibility of hazardous reactions

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYRALDEHYDE

Revision date: 07.12.2022

Product code: 222000

Page 6 of 10

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

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

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
78-84-2	NATURAL ISOBUTYRALDEHYDE				
	oral	LD50 mg/kg	3730	Rat	REACH registration OECD 401
	dermal	LD50 mg/kg	5670	Rabbit	Gestis
	inhalation (4 h) vapour	LC50 mg/l	>23,6	Rat	REACH registration OECD 403

Irritation and corrosivity

Causes serious eye irritation.

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

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.

SECTION 12: Ecological information

12.1. Toxicity

The product is not: Ecotoxic.

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYRALDEHYDE

Revision date: 07.12.2022

Product code: 222000

Page 7 of 10

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
78-84-2	NATURAL ISOBUTYRALDEHYDE					
	Acute fish toxicity	LC50	23 mg/l	96 h	Pimephales promelas (fathead minnow)	REACH registration
	Acute algae toxicity	ErC50	84 mg/l	72 h	Desmodesmus subspicatus	REACH registration DIN 38412 Part 9
	Acute crustacea toxicity	EC50	277 mg/l	48 h	Daphnia magna (Big water flea)	REACH registration EU Method C.2

12.2. Persistence and degradability

The product has not been tested.

CAS No	Chemical name				
	Method	Value	d	Source	
	Evaluation				
78-84-2	NATURAL ISOBUTYRALDEHYDE				
	OECD 301C	80 - 90%	14		
	Readily biodegradable (according to OECD criteria).				

12.3. Bioaccumulative potential

The product has not been tested.

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
78-84-2	NATURAL ISOBUTYRALDEHYDE	0,77

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

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYRALDEHYDE

Revision date: 07.12.2022

Product code: 222000

Page 8 of 10

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

Wash with plenty of water. Completely emptied packages can be recycled.

SECTION 14: Transport information

Land transport (ADR/RID)

14.1. UN number or ID number: UN 2045
14.2. UN proper shipping name: ISOBUTYRALDEHYDE (ISOBUTYL ALDEHYDE)
14.3. Transport hazard class(es): 3
14.4. Packing group: II
 Hazard label: 3



Classification code: F1
 Limited quantity: 1 L
 Excepted quantity: E2
 Transport category: 2
 Hazard No: 33
 Tunnel restriction code: D/E

Other applicable information (land transport)

E2

Inland waterways transport (ADN)

14.1. UN number or ID number: UN 2045
14.2. UN proper shipping name: ISOBUTYL ALDEHYDE (ISOBUTYRALDEHYDE)
14.3. Transport hazard class(es): 3
14.4. Packing group: II
 Hazard label: 3



Classification code: F1
 Limited quantity: 1 L
 Excepted quantity: E2

Other applicable information (inland waterways transport)

E2

Marine transport (IMDG)

14.1. UN number or ID number: UN 2045
14.2. UN proper shipping name: ISOBUTYL ALDEHYDE (ISOBUTYRALDEHYDE)
14.3. Transport hazard class(es): 3
14.4. Packing group: II
 Hazard label: 3



Special Provisions: -
 Limited quantity: 1 L
 Excepted quantity: E2

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYRALDEHYDE

Revision date: 07.12.2022

Product code: 222000

Page 9 of 10

EmS: F-E, S-D

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number: UN 2045
14.2. UN proper shipping name: ISOBUTYRALDEHYDE
14.3. Transport hazard class(es): 3
14.4. Packing group: II
 Hazard label: 3



Limited quantity Passenger: 1 L
 Passenger LQ: Y341
 Excepted quantity: E2
 IATA-packing instructions - Passenger: 353
 IATA-max. quantity - Passenger: 5 L
 IATA-packing instructions - Cargo: 364
 IATA-max. quantity - Cargo: 60 L

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

Warning: Combustible liquid.

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

2010/75/EU (VOC): 100 % (790 g/l)

2004/42/EC (VOC): 100 % (790 g/l)

Information according to 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).

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

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): 1,2,3,4,5,6,7,8,9,10,11,13,14,15,16.

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)

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYRALDEHYDE

Revision date: 07.12.2022

Product code: 222000

Page 10 of 10

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)

H225	Highly flammable liquid and vapour.
H319	Causes serious eye irritation.

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.