

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOVALERALDEHYDE

Revision date: 07.02.2024

Product code: 269200

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

1.1. Product identifier

NATURAL ISOVALERALDEHYDE

Substance name: NATURAL ISOVALERALDEHYDE
 CAS No: 590-86-3
 EC No: 209-691-5

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:	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. 2; H225
 Eye Irrit. 2; H319
 Skin Sens. 1; H317
 STOT SE 3; H335
 Aquatic Chronic 2; H411

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.
H317	May cause an allergic skin reaction.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H411	Toxic to aquatic life with long lasting effects.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No

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<p>P273 P280 P391 P403+P235</p>	<p>smoking. Avoid release to the environment. Wear protective gloves/protective clothing/eye protection/face protection/hearing protection. Collect spillage. Store in a well-ventilated place. Keep cool.</p>
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2.3. Other hazards

This substance is not listed as Substance of Very High Concern (SVHC) in the Candidate List according to REACH, Article 59. This substance is not identified as SVHC (substance of very high concern) and is not subject to authorisation according to Annex XIV of REACH.

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula:	C ₅ H ₁₀ O
Molecular weight:	86,13 g/mol

Relevant ingredients

CAS No	Chemical name	Quantity
	EC No	
	Index No	
	REACH No	
	Classification (Regulation (EC) No 1272/2008)	
590-86-3	NATURAL ISOVALERALDEHYDE	100 %
	209-691-5	
	Flam. Liq. 2, Eye Irrit. 2, Skin Sens. 1, STOT SE 3, Aquatic Chronic 2; H225 H319 H317 H335 H411	

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	
590-86-3	209-691-5	NATURAL ISOVALERALDEHYDE	100 %
		inhalation: LC50 = 42,7 mg/l (vapours); dermal: LD50 = 2534 mg/kg; oral: LD50 = 5740 mg/kg	

SECTION 4: First aid measures

4.1. Description of first aid measures

After inhalation

Provide fresh air. When in doubt or if symptoms are observed, get medical advice.

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. Medical treatment necessary.

After contact with eyes

After contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately.

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

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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. Heating causes rise in pressure with risk of bursting.

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. Provide adequate ventilation.

For emergency responders

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

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

Ventilate affected area.

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

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

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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)

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

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.

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 .

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	Liquid
Colour:	
Melting point/freezing point:	-51 °C
Boiling point or initial boiling point and boiling range:	92 °C
Flammability:	not determined
Lower explosion limits:	1,4 vol. %
Upper explosion limits:	5,6 vol. %
Flash point:	-1 °C
Auto-ignition temperature:	207 °C
Decomposition temperature:	not determined
pH-Value (at 20 °C):	3,1

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Viscosity / kinematic: (at 40 °C)	<6,9 mm ² /s
Water solubility: (at 20 °C)	15 g/l
Solubility in other solvents not determined	
Partition coefficient n-octanol/water:	1,5
Vapour pressure: (at 20 °C)	61 hPa
Density (at 20 °C):	0,80 g/cm ³
Relative vapour density: (at 20 °C)	2,97
Particle characteristics:	not applicable

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

The product is not: Explosive.

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)	0,69 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

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.

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CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
590-86-3	NATURAL ISOVALERALDEHYDE				
	oral	LD50 mg/kg	5740	Rat	REACH Dossier OECD 401
	dermal	LD50 mg/kg	2534	Rabbit	REACH Dossier OECD 402
	inhalation (4 h) vapour	LC50	42,7 mg/l	Rat	REACH Dossier OECD 403

Irritation and corrosivity

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

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

Sensitising effects

May cause an allergic skin reaction. (NATURAL ISOVALERALDEHYDE)

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

May cause respiratory irritation. (NATURAL ISOVALERALDEHYDE)

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.

Other information

This substance is classified as hazardous according to Regulation (EC) No 1272 (2008).

SECTION 12: Ecological information

12.1. Toxicity

Toxic to aquatic life with long lasting effects.

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
590-86-3	NATURAL ISOVALERALDEHYDE					
	Acute fish toxicity	LC50 mg/l	3,25	96 h Pimephales promelas (fathead minnow)	REACH Dossier	OECD 203
	Acute algae toxicity	ErC50	113 mg/l	72 h Desmodesmus subspicatus	REACH Dossier	German Industrial Standard DIN 38412,
	Acute crustacea toxicity	EC50	177 mg/l	48 h Daphnia magna (Big water flea)	REACH Dossier	Directive 79/831 EEC, C2

12.2. Persistence and degradability

The product has not been tested.

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CAS No	Chemical name			
	Method	Value	d	Source
	Evaluation			
590-86-3	NATURAL ISOVALERALDEHYDE			
	OECD 301D	49,5%	28	REACH Dossier
	Not readily biodegradable (according to OECD criteria)			
	OECD 301D	43,6%	20	REACH Dossier
	Not readily biodegradable (according to OECD criteria)			
	OECD 301D	36,9%	5	REACH Dossier
	Not 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
590-86-3	NATURAL ISOVALERALDEHYDE	1,5

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.

No information available.

12.7. Other adverse effects

No information available.

Further information

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal recommendations

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil. 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

Non-contaminated packages may be recycled. Handle contaminated packages in the same way as the substance itself.

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SECTION 14: Transport information

Land transport (ADR/RID)

14.1. UN number or ID number: UN 2058
14.2. UN proper shipping name: VALERALDEHYDE
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 2058
14.2. UN proper shipping name: VALERALDEHYDE
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 2058
14.2. UN proper shipping name: VALERALDEHYDE
14.3. Transport hazard class(es): 3
14.4. Packing group: II
 Hazard label: 3



Special Provisions: -
 Limited quantity: 1 L
 Excepted quantity: E2
 EmS: F-E, S-D

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number: UN 2058
14.2. UN proper shipping name: VALERALDEHYDE
14.3. Transport hazard class(es): 3
14.4. Packing group: II

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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: Yes



Danger releasing substance: ISOVALERALDEHYD

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 40

Directive 2010/75/EU on industrial emissions: 100 % (800 g/l)

Directive 2004/42/EC on VOC in paints and varnishes: 100 % (800 g/l)

Information according to Directive 2012/18/EU (SEVESO III): E2 Hazardous to the Aquatic Environment

Additional information: P5c

Additional information

To follow: 850/2004/EC, 79/117/EEC, 689/2008/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): 2 - obviously hazardous to water

Skin resorption/Sensitization: Causes allergic hypersensitivity reactions.

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): 1,2,4,5,6,7,8,9,10,11,12,13,14,15,16.

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Abbreviations and acronyms

Flam. Liq: Flammable liquid
Eye Irrit: Eye irritation
Skin Sens: Skin sensitisation
STOT SE: Specific target organ toxicity - single exposure
Aquatic Chronic: Chronic aquatic hazard
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>
EC/EEC: European Community/European Economic Community
EU: European Union
M-factor: Multiplying factor
IATA: International Air Transport Association
DGR: Dangerous Goods Regulations
ICAO: International Civil Aviation Organization
TI: Technical Instructions
VOC: volatile organic compound
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)

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H225	Highly flammable liquid and vapour.
H317	May cause an allergic skin reaction.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H411	Toxic to aquatic life with long lasting effects.

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.