

Safety Data Sheet

according to 29 CFR 1910.1200(g)

NATURAL ISOVALERALDEHYDE

Revision date: 02/07/2024

Product code: 269200US

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1. Identification

Product identifier

NATURAL ISOVALERALDEHYDE

Substance name: NATURAL ISOVALERALDEHYDE
CAS No: 590-86-3

Recommended use of the chemical and restrictions on use

Use of the substance/mixture

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

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	

Emergency phone number: +49 2822 68561 99

2. Hazard(s) identification

Classification of the chemical

29 CFR Part 1910.1200

Flammable liquids: Flam. Liq. 2
Serious eye damage/eye irritation: Eye Irrit. 2
Respiratory or skin sensitization: Skin Sens. 1
Specific target organ toxicity single exposure: STOT SE 3 (respiratory tract irritation)
Hazardous to the aquatic environment: Aquatic Acute 2
Hazardous to the aquatic environment: Aquatic Chronic 2

Label elements

29 CFR Part 1910.1200

Signal word: Danger

Pictograms:



Hazard statements

Highly flammable liquid and vapor
May cause an allergic skin reaction
Causes serious eye irritation
May cause respiratory irritation

Precautionary statements

Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
Keep container tightly closed.
Ground/bond container and receiving equipment.
Use explosion-proof electrical/ventilating/lighting equipment.
Use only non-sparking tools.

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Take precautionary measures against static discharge.
 Avoid breathing dust/fume/gas/mist/vapors/spray.
 Wash hands thoroughly after handling.
 Use only outdoors or in a well-ventilated area.
 Contaminated work clothing must not be allowed out of the workplace.
 Wear protective gloves/protective clothing/eye protection/face protection.
 If on skin: Wash with plenty of Water and soap.
 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
 If skin irritation or rash occurs: Get medical advice/attention.
 Wash contaminated clothing before reuse.
 If inhaled: Remove person to fresh air and keep comfortable for breathing.
 Call a poison center/doctor if you feel unwell.
 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.
 Continue rinsing.
 If eye irritation persists: Get medical advice/attention.
 Keep container tightly closed.
 Store in a well-ventilated place. Keep cool.
 Store locked up.
 Dispose of contents/container to Organic waste.

3. Composition/information on ingredients

Substances

Sum formula: C5 H10 O
 Molecular weight: 86,13 g/mol

Relevant ingredients

CAS No	Components	Quantity
590-86-3	NATURAL ISOVALERALDEHYDE	100 %

4. First-aid measures

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.

Most important symptoms and effects, both acute and delayed

No information available.

Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

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

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Specific hazards arising from the chemical

Highly flammable. Vapors may form explosive mixtures with air. Heating causes rise in pressure with risk of bursting.

Special protective equipment and precautions for fire-fighters

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/vapors/mists with water spray jet. Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.

6. Accidental release measures

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.

Environmental precautions

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

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.

Reference to other sections

Safe handling: see section 7

Personal protection equipment (PPE): see section 8

Disposal: see section 13

7. Handling and storage

Precautions for safe handling

Advice on safe handling

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

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges.

Vapors may 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.

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 exhaust 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.

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Hints on joint storage

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

8. Exposure controls/personal protection

Control parameters

Exposure controls



Appropriate engineering controls

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe gas/fume/vapor/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 .

9. Physical and chemical properties

Information on basic physical and chemical properties

Physical state:	Liquid
Color:	Colourless to pale yellow
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
Viscosity / kinematic: (at 40 °C)	<6,9 mm²/s
Water solubility: (at 20 °C)	15 g/l
Solubility in other solvents	not determined

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Partition coefficient n-octanol/water: 1,5
Vapor pressure: 61 hPa
(at 20 °C)
Density (at 20 °C): 0,80 g/cm³
Relative vapour density: 2,97
(at 20 °C)
Particle characteristics: not applicable

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: 0,69 mPa·s
(at 20 °C)

10. Stability and reactivity

Reactivity

Highly flammable.

Chemical stability

The product is stable under storage at normal ambient temperatures.

Possibility of hazardous reactions

No known hazardous reactions.

Conditions to avoid

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

Incompatible materials

No information available.

Hazardous decomposition products

No known hazardous decomposition products.

11. Toxicological information

Information on toxicological effects

Acute toxicity

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

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

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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.

Sensitizing 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.

Specific target organ toxicity (STOT) - single exposure

May cause respiratory irritation (NATURAL ISOVALERALDEHYDE)

Specific target organ toxicity (STOT) - repeated exposure

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

Carcinogenicity (OSHA): Not listed.

Carcinogenicity (IARC): Not listed.

Carcinogenicity (NTP): Not listed.

Aspiration hazard

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

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).

12. Ecological information

Ecotoxicity

Toxic to aquatic life with long lasting effects.

CAS No	Components					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
590-86-3	NATURAL ISOVALERALDEHYDE					
	Acute fish toxicity	LC50 3,25 mg/l	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

Persistence and degradability

The product has not been tested.

Bioaccumulative potential

The product has not been tested.

Partition coefficient n-octanol/water

CAS No	Components	Log Pow
590-86-3	NATURAL ISOVALERALDEHYDE	1,5

Mobility in soil

The product has not been tested.

Endocrine disrupting properties

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

No information available.

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.

13. Disposal considerations

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.

Contaminated packaging

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

14. Transport information

U.S. DOT 49 CFR 172.101

UN number or ID number:

UN 2058

Proper shipping name:

VALERALDEHYDE

Transport hazard class(es):

3

Packing group:

II

Hazard label:

3



Marine transport (IMDG)

UN number or ID number:

UN 2058

UN proper shipping name:

VALERALDEHYDE

Transport hazard class(es):

3

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)

UN number or ID number:

UN 2058

UN proper shipping name:

VALERALDEHYDE

Transport hazard class(es):

3

Packing group:

II

Hazard label:

3



Limited quantity Passenger:

1 L

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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

Environmental hazards

ENVIRONMENTALLY HAZARDOUS: Yes



Danger releasing substance: ISOVALERALDEHYD

Special precautions for user

Warning: Combustible liquid.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

not applicable

15. Regulatory information

U.S. Regulations

National regulatory information

SARA Section 311/312 Hazards:

NATURAL ISOVALERALDEHYDE (590-86-3): Fire hazard, Immediate (acute) health hazard

State Regulations

Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65, State of California)

This product can not expose you to chemicals known to the State of California to cause cancer, birth defects or other reproductive harm.

16. Other information

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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%
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: Multiplication 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).

Other data

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.