

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL 1-OCTANOL

Revision date: 01.06.2023

Product code: 280000

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

1.1. Product identifier

NATURAL 1-OCTANOL

Substance name:	NATURAL 1-OCTANOL
CAS No:	111-87-5
EC No:	203-917-6

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

Eye Irrit. 2; H319
Aquatic Chronic 3; H412

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Warning

Pictograms:



Hazard statements

H319	Causes serious eye irritation.
H412	Harmful to aquatic life with long lasting effects.

Precautionary statements

P264	Wash thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337+P313	If eye irritation persists: Get medical advice/attention.

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Dispose of contents/container to .

2.3. Other hazards

No information available.

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula: C₈ H₁₈ O

Molecular weight: 130,23

Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
111-87-5	NATURAL 1-OCTANOL			100 %
	203-917-6			
	Eye Irrit. 2, Aquatic Chronic 3; H319 H412			

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	
111-87-5	203-917-6	NATURAL 1-OCTANOL	100 %
	dermal: LD50 = >5000 mg/kg; oral: LD50 = >5000 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

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

5.1. Extinguishing media

Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings.

5.2. Special hazards arising from the substance or mixture

Non-flammable. Vapours can form explosive mixtures with air.

5.3. Advice for firefighters

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

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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

Provide adequate ventilation. 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 to enter into surface water or drains.

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

No special fire protection measures are necessary.

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.

Hints on joint storage

No special measures are necessary.

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

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DNEL/DMEL values

CAS No	Name of agent		
DNEL type	Exposure route	Effect	Value
111-87-5	NATURAL 1-OCTANOL		
Worker DNEL, long-term	inhalation	systemic	176 mg/m ³
Worker DNEL, long-term	inhalation	local	106 mg/m ³
Worker DNEL, long-term	dermal	systemic	50 mg/kg bw/day
Worker DNEL, long-term	dermal	local	0,190 mg/cm ²
Consumer DNEL, long-term	inhalation	systemic	43,5 mg/m ³
Consumer DNEL, long-term	dermal	systemic	25 mg/kg bw/day
Consumer DNEL, long-term	dermal	local	0,067 mg/cm ²
Consumer DNEL, long-term	oral	systemic	12,5 mg/kg bw/day

PNEC values

CAS No	Name of agent	
Environmental compartment	Value	
111-87-5	NATURAL 1-OCTANOL	
Freshwater	0,2 mg/l	
Marine water	0,02 mg/l	
Freshwater sediment	2,1 mg/kg	
Marine sediment	0,21 mg/kg	
Soil	0,26 mg/kg	

8.2. Exposure controls



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

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:

colourless

Melting point/freezing point:

-15 °C

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Boiling point or initial boiling point and boiling range:	194 °C
Flammability:	not determined
Lower explosion limits:	not determined
Upper explosion limits:	not determined
Flash point:	87 °C
Auto-ignition temperature:	294 °C
Decomposition temperature:	not determined
pH-Value:	not determined
Viscosity / kinematic: (at 40 °C)	5,6 mm ² /s
Water solubility: (at 25 °C)	0,1 g/L
Solubility in other solvents	not determined
Partition coefficient n-octanol/water:	3,5
Vapour pressure: (at 20 °C)	0,052 hPa
Vapour pressure: (at 50 °C)	0,95 hPa
Density (at 20 °C):	0,83 g/cm ³
Relative vapour density: (at 20 °C)	4,5

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) 9 mPa·s

SECTION 10: Stability and reactivity

10.1. Reactivity

No hazardous reaction when handled and stored according to provisions.

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

none

10.5. Incompatible materials

No information available.

10.6. Hazardous decomposition products

No known hazardous decomposition products.

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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
111-87-5	NATURAL 1-OCTANOL				
	oral	LD50 >5000 mg/kg	Rat	REACH Registration	OECD 401
	dermal	LD50 >5000 mg/kg	Rat	REACH Registration	EPA OPPTS 870.1200

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.

11.2. Information on other hazards

Endocrine disrupting properties

No information available.

Further information

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

SECTION 12: Ecological information

12.1. Toxicity

Harmful to aquatic life with long lasting effects.

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CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
111-87-5	NATURAL 1-OCTANOL					
	Acute fish toxicity	LC50 mg/l	13,3	96 h	Pimephales promelas (fathead minnow)	REACH Registration OECD 203
	Acute algae toxicity	ErC50	6,5 mg/l		Desmodesmus subspicatus	REACH Registration OECD 201
	Acute crustacea toxicity	EC50	20 mg/l	48 h	Daphnia magna (Big water flea)	REACH Registration OECD 202
	Fish toxicity	NOEC	1,5 mg/l	7 d	Pimephales promelas (fathead minnow)	REACH Registration
	Crustacea toxicity	NOEC	1 mg/l	21 d	Daphnia magna (Big water flea)	REACH Registration OECD 211
	Acute bacteria toxicity	(EC50 mg/l)	350	3 h	Activated sludge	REACH Registration OECD 209

12.2. Persistence and degradability

The product has not been tested.

CAS No	Chemical name			
	Method	Value	d	Source
	Evaluation			
111-87-5	NATURAL 1-OCTANOL			
	OECD 301B	92%	28	REACH Registration
	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
111-87-5	NATURAL 1-OCTANOL	3,5

BCF

CAS No	Chemical name	BCF	Species	Source
111-87-5	NATURAL 1-OCTANOL	9,1		

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

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

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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.

SECTION 14: Transport information

Land transport (ADR/RID)

<u>14.1. UN number or ID number:</u>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

Inland waterways transport (ADN)

<u>14.1. UN number or ID number:</u>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

Marine transport (IMDG)

<u>14.1. UN number or ID number:</u>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

Air transport (ICAO-TI/IATA-DGR)

<u>14.1. UN number or ID number:</u>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

No information available.

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

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2004/42/EC (VOC): 100 % (830 g/l)
Information according to 2012/18/EU (SEVESO III): Not subject to 2012/18/EU (SEVESO III):

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

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)
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

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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)

H319 Causes serious eye irritation.
H412 Harmful 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.