

## Safety Data Sheet

according to Regulation (EC) No 1907/2006

### NATURAL 3-MERCAPTOHEXANOL 0.1% IN ETHANOL

Revision date: 18.11.2022

Product code: 385020

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

##### 1.1. Product identifier

NATURAL 3-MERCAPTOHEXANOL 0.1% IN ETHANOL

UFI: TQ9D-S373-U104-1RE2

##### 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.  
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing

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<p>P303+P361+P353 P305+P351+P338 P337+P313 P370+P378 P403+P235 P501</p>	<p>protection. IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower. 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. In case of fire: Use Carbon dioxide (CO<sub>2</sub>) / Foam / Extinguishing powder to extinguish. Store in a well-ventilated place. Keep cool. Dispose of contents/container to .</p>
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#### 2.3. Other hazards

No information available.

### SECTION 3: Composition/information on ingredients

#### 3.2. Mixtures

##### Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
64-17-5	ethanol, ethyl alcohol			99,5 - 99,9 %
	200-578-6	603-002-00-5	01-2119457610-43	
	Flam. Liq. 2, Eye Irrit. 2; H225 H319			
51755-83-0	NATURAL 3-MERCAPTOHEXANOL			0,1 - 0,5 %
	440-730-0			
	Aquatic Chronic 2; 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	
64-17-5	200-578-6	ethanol, ethyl alcohol	99,5 - 99,9 %
	inhalation: LC50 = 121 mg/l (vapours); dermal: LD50 = 17100 mg/kg; oral: LD50 = 10470 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

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.

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#### SECTION 5: Firefighting measures

##### 5.1. Extinguishing media

###### **Suitable extinguishing media**

Water spray jet, Carbon dioxide (CO<sub>2</sub>), 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. 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

#### 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**

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 in a cool, well-ventilated place. Keep away from heat, hot surfaces, sparks,

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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

##### DNEL/DMEL values

CAS No	Name of agent	Exposure route	Effect	Value
64-17-5	ethanol, ethyl alcohol			
Worker DNEL, long-term		inhalation	systemic	380-950 mg/m <sup>3</sup>
Worker DNEL, long-term		dermal	systemic	343 mg/kg bw/day
Consumer DNEL, long-term		inhalation	systemic	114 mg/m <sup>3</sup>
Consumer DNEL, long-term		dermal	systemic	206 mg/kg bw/day
Consumer DNEL, long-term		oral	systemic	87 mg/kg bw/day
Worker DNEL, acute		inhalation	local	1900 mg/m <sup>3</sup>
Consumer DNEL, acute		inhalation	local	950 mg/m <sup>3</sup>

##### PNEC values

CAS No	Name of agent	Value
64-17-5	ethanol, ethyl alcohol	
Freshwater		0,96 mg/l
Marine water		0,79 mg/l
Freshwater sediment		3,6 mg/kg
Marine sediment		2,9 mg/kg
Secondary poisoning		380 mg/kg
Micro-organisms in sewage treatment plants (STP)		580 mg/l
Soil		0,63 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.

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#### **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:	colourless	
Melting point/freezing point:		not determined
Boiling point or initial boiling point and boiling range:		> 78 °C
Flammability		
Solid/liquid:		not applicable
Gas:		not applicable
Lower explosion limits:		3,1 vol. %
Upper explosion limits:		27,7 vol. %
Flash point:		> 13 °C
Auto-ignition temperature:		368 °C
Decomposition temperature:		not determined
pH-Value:		not determined
Water solubility:		Yes.
Solubility in other solvents		
not determined		
Partition coefficient n-octanol/water:		not determined
Vapour pressure:		58 hPa
(at 20 °C)		
Vapour pressure:		293 hPa
(at 50 °C)		
Density (at 20 °C):		0,79 g/cm <sup>3</sup>
Relative vapour density:		not determined

#### **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: 99,90 %

Solid content: not determined

### 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**

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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
64-17-5	ethanol, ethyl alcohol				
	oral	LD50 mg/kg	10470	Rat	REACH Dossier OECD 401
	dermal	LD50 mg/kg	17100	Rabbit	REACH Dossier
	inhalation (4 h) vapour	LC50	121 mg/l	Rat	REACH Dossier 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.

#### **11.2. Information on other hazards**

##### **Endocrine disrupting properties**

The product has not been tested.

##### **Further information**

The mixture is classified as hazardous according to regulation (EC) No 1272/2008 [CLP].

### **SECTION 12: Ecological information**

#### **12.1. Toxicity**

The product is not: Ecotoxic.

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CAS No	Chemical name					
	Aquatic toxicity	Dose	[h]   [d]	Species	Source	Method
64-17-5	ethanol, ethyl alcohol					
	Acute fish toxicity	LC50 mg/l	14200	96 h	Pimephales promelas (fathead minnow)	REACH Dossier US EPA method E03-05
	Acute algae toxicity	ErC50	275 mg/l	72 h	Chlorella vulgaris	REACH Dossier OECD 201
	Acute crustacea toxicity	EC50 mg/l	5012	48 h	Ceriodaphnia spec	REACH Dossier ASTM E729-80
	Fish toxicity	NOEC	250 mg/l	5 d	Danio rerio (zebrafish)	REACH Dossier OECD 212
	Crustacea toxicity	NOEC	9,6 mg/l	9 d	Daphnia magna	
	Acute bacteria toxicity	(EC50 mg/l)	>1000	3 h	Activated sludge	REACH Dossier OECD 209
51755-83-0	NATURAL 3-MERCAPTOHEXANOL					
	Acute crustacea toxicity	EC50	8,5 mg/l	48 h	Daphnia magna (Big water flea)	REACH registration OECD 202

#### 12.2. Persistence and degradability

The product has not been tested.

CAS No	Chemical name			
	Method	Value	d	Source
	Evaluation			
64-17-5	ethanol, ethyl alcohol			
	OECD 301B	95%	28	REACH Dossier
	Readily biodegradable (according to OECD criteria).			
	OECD 301B	84%	20	REACH Dossier
	Readily biodegradable (according to OECD criteria).			
	OECD 301B	74%	5	REACH Dossier
	Readily biodegradable (according to OECD criteria).			
51755-83-0	NATURAL 3-MERCAPTOHEXANOL			
	OECD 301D	10%	28	REACH registration
	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
64-17-5	ethanol, ethyl alcohol	-0,3
51755-83-0	NATURAL 3-MERCAPTOHEXANOL	1,63

#### BCF

CAS No	Chemical name	BCF	Species	Source
64-17-5	ethanol, ethyl alcohol	1-4,5	Cyprinus carpio (Common Carp)	REACH Registration

#### 12.4. Mobility in soil

The product has not been tested.

#### 12.5. Results of PBT and vPvB assessment

The substances in the mixture do not meet the PBT/vPvB criteria according to REACH, annex XIII.

The product has not been tested.

#### 12.6. Endocrine disrupting properties

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This product does not contain a substance that has endocrine disrupting properties with respect to non-target organisms as no components meets the criteria.

#### **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**

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

### **SECTION 14: Transport information**

#### **Land transport (ADR/RID)**

<b><u>14.1. UN number or ID number:</u></b>	UN 1170
<b><u>14.2. UN proper shipping name:</u></b>	ETHANOL SOLUTION (ETHYL ALCOHOL SOLUTION)
<b><u>14.3. Transport hazard class(es):</u></b>	3
<b><u>14.4. Packing group:</u></b>	II
Hazard label:	3



Classification code:	F1
Special Provisions:	144 601
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)**

<b><u>14.1. UN number or ID number:</u></b>	UN 1170
<b><u>14.2. UN proper shipping name:</u></b>	ETHANOL SOLUTION (ETHYL ALCOHOL SOLUTION)
<b><u>14.3. Transport hazard class(es):</u></b>	3
<b><u>14.4. Packing group:</u></b>	II
Hazard label:	3



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Classification code: F1  
 Special Provisions: 144 601  
 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 1170  
**14.2. UN proper shipping name:** ETHANOL SOLUTION (ETHYL ALCOHOL SOLUTION)  
**14.3. Transport hazard class(es):** 3  
**14.4. Packing group:** II  
 Hazard label: 3



Special Provisions: 144  
 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 1170  
**14.2. UN proper shipping name:** ETHANOL SOLUTION  
**14.3. Transport hazard class(es):** 3  
**14.4. Packing group:** II  
 Hazard label: 3



Special Provisions: A3 A58 A180  
 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

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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, 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

Chemical safety assessments for substances in this mixture were not 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.

#### 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

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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).

**Classification for mixtures and used evaluation method according to regulation (EC) No 1272/2008 [CLP]**

Classification	Classification procedure
Flam. Liq. 2; H225	On basis of test data
Eye Irrit. 2; H319	Calculation method

**Relevant H and EUH statements (number and full text)**

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

*(The data for the hazardous ingredients were taken respectively from the last version of the sub-contractor's safety data sheet.)*