

# Safety Data Sheet

according to Regulation (EC) No 1907/2006

## NATURAL 3-MERCAPTOHEXANOL

Revision date: 23.07.2021

Product code: 385000

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

#### 1.1. Product identifier

NATURAL 3-MERCAPTOHEXANOL

Substance name: NATURAL 3-MERCAPTOHEXANOL  
CAS No: 51755-83-0  
EC No: 440-730-0  
UFI: RY7D-N3E5-Q107-TWRS

#### 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  
e-mail: info@axxence.com  
Contact person: Andreas Goertz  
e-mail: andreas.goertz@axxence.com  
Internet: www.axxence.de  
Responsible Department: QM - Regulatory Affairs

Telefax: + 49 2822 68561 39

Telephone: + 49 2822 68561 37

#### 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

Aquatic Chronic 2; H411

Full text of hazard statements: see SECTION 16.

#### 2.2. Label elements

##### Regulation (EC) No 1272/2008

##### Pictograms:



##### Hazard statements

H411 Toxic to aquatic life with long lasting effects.

##### Precautionary statements

P273 Avoid release to the environment.  
P391 Collect spillage.  
P501 Dispose of contents/container to .

#### 2.3. Other hazards

No information available.

### SECTION 3: Composition/information on ingredients

#### 3.1. Substances

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Sum formula: C<sub>6</sub> H<sub>14</sub> O S

Molecular weight: 134,24

### Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
51755-83-0	NATURAL 3-MERCAPTOHEXANOL			100 %
	440-730-0			
	Aquatic Chronic 2; H411			

Full text of H and EUH statements: see section 16.

## 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

Rinse mouth immediately and drink 1 glass of water. Rinse mouth immediately and drink plenty 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.

### 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

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

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### 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

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

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

### 8.2. Exposure controls

#### Individual protection measures, such as personal protective equipment

##### Eye/face protection

Wear eye/face protection.

##### 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:

Melting point/freezing point:

-55 °C

Boiling point or initial boiling point and boiling range:

245 °C

Flammability

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Solid/liquid:	not applicable
Gas:	not applicable
Lower explosion limits:	not determined
Upper explosion limits:	not determined
Flash point:	108 °C
Auto-ignition temperature:	245 °C
Decomposition temperature:	not determined
pH-Value:	not determined
Water solubility:	6,8 g/L
(at 20 °C)	
Solubility in other solvents	
not determined	
Partition coefficient n-octanol/water:	1,644
Vapour pressure:	6,3 hPa
(at 20 °C)	
Density (at 20 °C):	0,97 g/cm³
Relative vapour density:	not determined

### 9.2. Other information

#### Information with regard to physical hazard classes

##### Explosive properties

The product is not: Explosive. not explosive according to EU A.14

##### Self-ignition temperature

Solid:

not applicable

Gas:

not applicable

##### Oxidizing properties

The product is not: oxidising.

#### Other safety characteristics

Evaporation rate:

not determined

Solvent content:

0%

Solid content:

0%

## 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.

## 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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### Irritation and corrosivity

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.

## 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
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.

The product has not been tested.				
CAS No	Chemical name			
	Method	Value	d	Source
	Evaluation			
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
51755-83-0	NATURAL 3-MERCAPTOHEXANOL	1,63

### 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.

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### 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.

## SECTION 14: Transport information

### Land transport (ADR/RID)

#### 14.1. UN number or ID number:

UN 3082

#### 14.2. UN proper shipping name:

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.

#### 14.3. Transport hazard class(es):

9

#### 14.4. Packing group:

III

Hazard label:

9



Classification code:

M6

Special Provisions:

274 335 375 601

Limited quantity:

5 L

Excepted quantity:

E1

Transport category:

3

Hazard No:

90

Tunnel restriction code:

-

### Inland waterways transport (ADN)

#### 14.1. UN number or ID number:

UN 3082

#### 14.2. UN proper shipping name:

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.

#### 14.3. Transport hazard class(es):

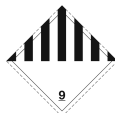
9

#### 14.4. Packing group:

III

Hazard label:

9



Classification code:

M6

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Special Provisions: 274 335 375 601  
 Limited quantity: 5 L  
 Excepted quantity: E1

### Marine transport (IMDG)

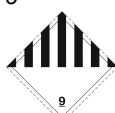
**14.1. UN number or ID number:** UN 3082  
**14.2. UN proper shipping name:** ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.  
**14.3. Transport hazard class(es):** 9  
**14.4. Packing group:** III  
 Hazard label: 9



Special Provisions: 274, 335, 969  
 Limited quantity: 5 L  
 Excepted quantity: E1  
 EmS: F-A, S-F

### Air transport (ICAO-TI/IATA-DGR)

**14.1. UN number or ID number:** UN 3082  
**14.2. UN proper shipping name:** ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.  
**14.3. Transport hazard class(es):** 9  
**14.4. Packing group:** III  
 Hazard label: 9



Special Provisions: A97 A158 A197 A215  
 Limited quantity Passenger: 30 kg G  
 Passenger LQ: Y964  
 Excepted quantity: E1  
 IATA-packing instructions - Passenger: 964  
 IATA-max. quantity - Passenger: 450 L  
 IATA-packing instructions - Cargo: 964  
 IATA-max. quantity - Cargo: 450 L

### 14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: Yes



Danger releasing substance: NATURAL 3-MERCAPTOHEXANOL

### 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

2010/75/EU (VOC): 100 % (970 g/l)

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2004/42/EC (VOC): 100 % (970 g/l)  
Information according to 2012/18/EU (SEVESO III): E2 Hazardous to the Aquatic Environment

### 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): 3 - highly 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): 1,2,4,5,6,7,9,11,12,14,15.

### 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>

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

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.

### Identified uses

No	Short title	LCS	SU	PC	PROC	ERC	AC	TF	Specification
1		-	4	28	-	-	-	-	Flavour

LCS: Life cycle stages

PC: Product categories

ERC: Environmental release categories

TF: Technical functions

SU: Sectors of use

PROC: Process categories

AC: Article categories