

according to UN GHS (ST/SG/AC.10/11/Rev.9)

#### **NATURAL 3-MERCAPTOHEXANOL**

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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

# 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 +49 2822 68561 99

number:

### **SECTION 2: Hazards identification**

### 2.1. Classification of the substance or mixture

### UN GHS (ST/SG/AC.10/11/Rev.9)

Acute toxicity: Acute Tox. 4 (oral)

Hazardous to the aquatic environment: Aquatic Acute 2 Hazardous to the aquatic environment: Aquatic Chronic 2

### 2.2. Label elements

### UN GHS (ST/SG/AC.10/11/Rev.9)

### 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

Sum formula: C6 H14 O S

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Molecular weight: 134,24

#### **Hazardous components**

CAS No	Chemical name	Quantity
	Classification (UN GHS (ST/SG/AC.10/11/Rev.9))	
51755-83-0	NATURAL 3-MERCAPTOHEXANOL	100 %
	Acute Tox. 4, Aquatic Acute 2, Aquatic Chronic 2; H302 H401 H411	

### **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. In case of eye irritation consult an ophthalmologist.

## After ingestion

Rinse mouth immediately and drink 1 glass of of water. Medical treatment necessary. 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.

### 5.3. Advice for firefighters

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

#### Additional information

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.





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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

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

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. 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



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Boiling point or initial boiling point and

245 °C

6,8 g/L

boiling range:

Flammability:

Lower explosion limits:

Upper explosion limits:

not determined

Upper explosion limits:

not determined

Flash point:

Auto-ignition temperature:

Decomposition temperature:

pH-Value:

not determined

not determined

Water solubility: (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

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 toxicological effects

### **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
51755-83-0	NATURAL 3-MERCAPTOHEXANOL				
	oral	LD50 <2000 mg/kg		Symrise Study	OECD 401

### 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.

#### **Further 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	
51755-83-0	NATURAL 3-MERCAPTOHEXANOL					
	Acute crustacea toxicity	EC50 8,5 mg/l	1 1	REACH registration	OECD 202	

# 12.2. Persistence and degradability

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.

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#### 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.

### Contaminated packaging

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

# **SECTION 14: Transport information**

## 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):

14.4. Packing group:

Hazard label:



Ш

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:



Special Provisions: A97 A158 A197 A215

Limited quantity Passenger: 30 kg G
Passenger LQ: Y964
Excepted quantity: E1

IATA-packing instructions - Passenger:964IATA-max. quantity - Passenger:450 LIATA-packing instructions - Cargo:964IATA-max. quantity - Cargo:450 L

### 14.5. Environmental hazards



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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**

### **National regulatory information**

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile

work protection guideline' (94/33/EC).

## **SECTION 16: Other information**

### Changes

This data sheet contains changes from the previous version in section(s): 2,4,5,6,7,9,11,14,15,16.

#### 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



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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).

### **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.