

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL 3-MERCAPTOHEXANOL

Revision date: 27.02.2023

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

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: Safety Team
E-mail: safety-documentation@axxence.com
Internet: www.axxence.de
Responsible Department: Safety Management

Telefax: + 49 2822 68561 39

Telephone: + 49 2822 68561 0

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

Acute Tox. 4; H302
Aquatic Chronic 2; H411

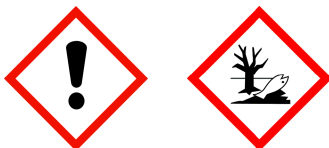
Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Warning

Pictograms:



Hazard statements

H302 Harmful if swallowed.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

P264 Wash hands thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P273 Avoid release to the environment.
P301+P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P330 Rinse mouth.
P391 Collect spillage.
P501 Dispose of contents/container to organic waste.

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2.3. Other hazards

No information available.

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula: C₆ H₁₄ O S
Molecular weight: 134,24 g/mol

Relevant ingredients

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			
	Acute Tox. 4, Aquatic Chronic 2; H302 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	
51755-83-0	440-730-0	NATURAL 3-MERCAPTOHEXANOL	100 %
	oral: LD50 = <2000 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

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 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.

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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.

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 protection/face protection.

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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:	not determined
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: (at 20 °C)	6,8 g/l
Solubility in other solvents	not determined
Partition coefficient n-octanol/water:	1,644
Vapour pressure: (at 20 °C)	6,3 hPa
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.

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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

Harmful if swallowed.

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
51755-83-0	NATURAL 3-MERCAPTOHEXANOL				
	oral	LD50 mg/kg	<2000	Symrise Study	OECD 401

Irritation and corrosivity

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

Serious eye damage/eye 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

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.

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.

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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.

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

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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):

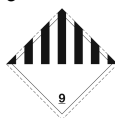
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14.4. Packing group:

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):

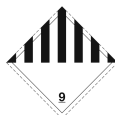
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14.4. Packing group:

III

Hazard label:

9



Classification code:

M6

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.

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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

Directive 2010/75/EU on industrial emissions:

100 % (970 g/l)

Directive 2004/42/EC on VOC in paints and varnishes:

100 % (970 g/l)

Information according to Directive 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): 1,2,4,5,6,7,9,11,14,15,16.

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Abbreviations and acronyms

Acute Tox: Acute toxicity
 Aquatic Chronic: Chronic aquatic hazard
 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>
 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)

H302 Harmful if swallowed.
 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.

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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