

# Safety Data Sheet

according to Regulation (EC) No 1907/2006

## NATURAL 4-MERCAPTO-4-METHYL-2- PENTANONE 1% IN ETHANOL

Revision date: 03.03.2025

Product code: 399710

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

#### 1.1. Product identifier

NATURAL 4-MERCAPTO-4-METHYL-2- PENTANONE 1% IN ETHANOL

UFI: FWYP-W4MQ-510Y-9KNT

#### 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:	Safety Team	Telephone: + 49 2822 68561 0
E-mail:	safety-documentation@axxence.com	
Internet:	www.axxence.de	
Responsible Department:	Safety Management	

#### 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 hands thoroughly after handling.  
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing

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P303+P361+P353	protection. IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
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.
P370+P378	In case of fire: Use Carbon dioxide (CO <sub>2</sub> ), Extinguishing powder, alcohol resistant foam to extinguish.
P403+P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/container to organic waste.

### 2.3. Other hazards

Contains no substances of very high concern (SVHC) which are included in the Candidate List according to Article 59 of REACH.

Contains no substances of very high concern (SVHC) which are subject to authorisation according to Annex XIV of REACH.

## SECTION 3: Composition/information on ingredients

### 3.2. Mixtures

#### Relevant ingredients

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
64-17-5	ethanol, ethyl alcohol			98,5 - 99,0 %
	200-578-6	603-002-00-5	01-2119457610-43	
	Flam. Liq. 2; Eye Irrit. 2; H225 H319			
19872-52-7	NATURAL 4-MERCAPTO-4-METHYL-2-PENTANONE			1,0 - 1,5 %
	243-386-8			
	Flam. Liq. 3; H226			

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	98,5 - 99,0 %
	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.

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### 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

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

#### 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.

### 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, open flames and other ignition sources. No smoking.

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### 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			
DNEL type		Exposure route	Effect	Value
64-17-5	ethanol, ethyl alcohol			
Worker DNEL, long-term		inhalation	systemic	380-950 mg/m³
Worker DNEL, long-term		dermal	systemic	343 mg/kg bw/day
Consumer DNEL, long-term		inhalation	systemic	114 mg/m³
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/m³
Consumer DNEL, acute		inhalation	local	950 mg/m³

#### PNEC values

CAS No	Name of agent		
Environmental compartment			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.

## 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:		not applicable
		not applicable
Lower explosion limits:		3,1 vol. %
Upper explosion limits:		27,7 vol. %
Flash point:		12 °C
Auto-ignition temperature:		363 °C
Decomposition temperature:		not determined
pH-Value (at 20 °C):		7
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:		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

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

##### Self-ignition temperature

Solid:

not applicable

Gas:

not applicable

##### Oxidizing properties

Not oxidising.

#### Other safety characteristics

Evaporation rate:	not determined
Solvent content:	99,00 %
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

No known hazardous reactions.

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### 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.

#### ATEmix calculated

ATE (oral) > 2000 mg/kg; ATE (dermal) > 2000 mg/kg; ATE (inhalation vapour) > 20 mg/l; ATE (inhalation dust/mist) > 5 mg/l

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
64-17-5	ethanol, ethyl alcohol				
	oral	LD50 mg/kg	10470	Rat	REACH Dossier
	dermal	LD50 mg/kg	17100	Rabbit	REACH Dossier
	inhalation (4 h) vapour	LC50	121 mg/l	Rat	REACH Dossier
					OECD 401
					OECD 403

#### Irritation and corrosivity

Serious eye damage/eye irritation: 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

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.

#### Additional information on tests

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

### 11.2. Information on other hazards

#### Endocrine disrupting properties

No information available.

## 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	REACH Dossier
	Acute bacteria toxicity	EC50 mg/l ( )	>1000	3 h	Activated sludge	REACH Dossier OECD 209

**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).			

**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
19872-52-7	NATURAL 4-MERCAPTO-4-METHYL-2-PENTANONE	1,432

**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**

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**

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

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### 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 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



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

#### Inland waterways transport (ADN)

**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



Classification code: F1  
Special Provisions: 144 601  
Limited quantity: 1 L



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Excepted quantity: 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

Restrictions on use (REACH, annex XVII):

Entry 3, Entry 40

Directive 2010/75/EU on industrial emissions: 99 % (782,1 g/l)

Directive 2004/42/EC on VOC in paints and varnishes: 100 % (790 g/l)

Information according to Directive 2012/18/EU (SEVESO III): P5c FLAMMABLE LIQUIDS

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### 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): 2 - obviously 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

Flam. Liq: Flammable liquid  
Eye Irrit: Eye irritation  
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>

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### 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.
H226	Flammable liquid and vapour.
H319	Causes serious eye irritation.

### 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 relevant ingredients were taken respectively from the last version of the sub-contractor's safety data sheet.)*