

Safety Data Sheet

according to Regulation (EC) No 1907/2006

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

Revision date: 03.03.2025

Product code: 399700

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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 PG

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

This mixture is not classified as hazardous in accordance with Regulation (EC) No 1272/2008.

2.2. Label elements

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)			
57-55-6	PROPYLENE GLYCOL			98,00-99,00 %
	200-338-0		01-2119456809-23	
19872-52-7	NATURAL 4-MERCAPTO-4-METHYL-2-PENTANONE			1,0-2,0 %
	243-386-8			
	Flam. Liq. 3; H226			

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

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Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
57-55-6	200-338-0	PROPYLENE GLYCOL	98,00-99,00 %
		dermal: LD50 = 20800 mg/kg; oral: LD50 = 22000 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.

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.

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

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

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

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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.

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
57-55-6	PROPYLENE GLYCOL			
Worker DNEL, long-term		inhalation	systemic	168 mg/m³
Worker DNEL, long-term		inhalation	local	10 mg/m³
Consumer DNEL, long-term		inhalation	systemic	50 mg/m³
Consumer DNEL, long-term		inhalation	local	10 mg/m³

PNEC values

CAS No	Name of agent	
Environmental compartment	Value	
57-55-6	PROPYLENE GLYCOL	
Freshwater	260 mg/l	
Freshwater (intermittent releases)	183 mg/l	
Marine water	26 mg/l	
Freshwater sediment	572 mg/kg	
Marine sediment	57,2 mg/kg	
Micro-organisms in sewage treatment plants (STP)	20000 mg/l	
Soil	50 mg/kg	

8.2. Exposure controls

Individual protection measures, such as personal protective equipment

Eye/face protection

Wear eye protection/face protection.

Hand protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four

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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:	colourless	
Melting point/freezing point:		not determined
Boiling point or initial boiling point and boiling range:		184 °C
Flammability:		not applicable
		not applicable
Lower explosion limits:		2,6 vol. %
Upper explosion limits:		12,6 vol. %
Flash point:		104 °C
Auto-ignition temperature:		420 °C
Decomposition temperature:		not determined
pH-Value:		not determined
Solubility in other solvents		
not determined		
Partition coefficient n-octanol/water:		not determined
Vapour pressure:		0,11 hPa
(at 20 °C)		
Vapour pressure:		0,17 hPa
(at 50 °C)		
Density (at 20 °C):		1,04 g/cm ³
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

No hazardous reaction when handled and stored according to provisions.

10.2. Chemical stability

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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.

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
57-55-6	PROPYLENE GLYCOL				
	oral	LD50 mg/kg	22000	Rat	REACH registration
	dermal	LD50 mg/kg	20800	Rabbit	GESTIS

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.

Additional information on tests

The mixture is classified as not 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

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The product is not: Ecotoxic.

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
57-55-6	PROPYLENE GLYCOL					
	Acute fish toxicity	LC50 mg/l	40613	96 h	Oncorhynchus mykiss (Rainbow trout)	REACH registration Guideline: Environment Canada (1990)
	Acute algae toxicity	ErC50 mg/l	19000	96 h	Pseudokirchneriella subcapitata	REACH registration OECD 201
	Acute crustacea toxicity	EC50 mg/l	18340	48 h	Ceriodaphnia spec	REACH registration EPA 600/4-90/0-27
	Fish toxicity	NOEC mg/l	11530	7 d	Pimephales promelas (fathead minnow)	REACH registration EPA 600/4-89/001
	Algae toxicity	NOEC mg/l	15000	14 d	Pseudokirchneriella subcapitata	REACH registration OECD 201
	Crustacea toxicity	NOEC mg/l	13020	7 d	Ceriodaphnia spec	REACH registration EPA 600/4-89/001
	Acute bacteria toxicity	EC50 mg/l ()	>20000	0 h	Pseudomonas putida	REACH registration German guideline:"Bewert ung wassergefahr

12.2. Persistence and degradability

The product has not been tested.

CAS No	Chemical name			
	Method	Value	d	Source
	Evaluation			
57-55-6	PROPYLENE GLYCOL			
	OECD 301F	98,3%	28	REACH registration
	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
57-55-6	PROPYLENE GLYCOL	-1,07
19872-52-7	NATURAL 4-MERCAPTO-4-METHYL-2-PENTANONE	1,432

BCF

CAS No	Chemical name	BCF	Species	Source
57-55-6	PROPYLENE GLYCOL	0,09		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.

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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

160306 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; off-specification batches and unused products; organic wastes other than those mentioned in 16 03 05

List of Wastes Code - used product

160306 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; off-specification batches and unused products; organic wastes other than those mentioned in 16 03 05

List of Wastes Code - contaminated packaging

150102 WASTE PACKAGING; ABSORBENTS, WIPING CLOTHS, FILTER MATERIALS AND PROTECTIVE CLOTHING NOT OTHERWISE SPECIFIED; packaging (including separately collected municipal packaging waste); plastic packaging

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:

No dangerous good in sense of this transport regulation.

14.2. UN proper shipping name:

No dangerous good in sense of this transport regulation.

14.3. Transport hazard class(es):

No dangerous good in sense of this transport regulation.

14.4. Packing group:

No dangerous good in sense of this transport regulation.

Inland waterways transport (ADN)

14.1. UN number or ID number:

No dangerous good in sense of this transport regulation.

14.2. UN proper shipping name:

No dangerous good in sense of this transport regulation.

14.3. Transport hazard class(es):

No dangerous good in sense of this transport regulation.

14.4. Packing group:

No dangerous good in sense of this transport regulation.

Marine transport (IMDG)

14.1. UN number or ID number:

No dangerous good in sense of this transport regulation.

14.2. UN proper shipping name:

No dangerous good in sense of this transport regulation.

14.3. Transport hazard class(es):

No dangerous good in sense of this transport regulation.

14.4. Packing group:

No dangerous good in sense of this transport regulation.

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number:

No dangerous good in sense of this transport regulation.

14.2. UN proper shipping name:

No dangerous good in sense of this transport regulation.

14.3. Transport hazard class(es):

No dangerous good in sense of this transport regulation.

14.4. Packing group:

No dangerous good in sense of this transport regulation.

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

No information available.

14.7. Maritime transport in bulk according to IMO instruments

not applicable

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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 40

Directive 2010/75/EU on industrial emissions: 99 % (1029,6 g/l)

Directive 2004/42/EC on VOC in paints and varnishes: 100 % (1040 g/l)

Information according to Directive 2012/18/EU (SEVESO III): Not subject to 2012/18/EU (SEVESO III)

Additional information

To follow: 850/2004/EC, 79/117/EEC, 689/2008/EC

National regulatory information

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

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Abbreviations and acronyms

Flam. Liq: Flammable liquid
 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>

Relevant H and EUH statements (number and full text)

H226 Flammable liquid and vapour.

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.)