

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL 3-MERCAPTO-2-METHYL-1-PENTANOL 1% IN TRIACETIN

Revision date: 25.03.2025

Product code: 399610

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

1.1. Product identifier

NATURAL 3-MERCAPTO-2-METHYL-1-PENTANOL 1% IN TRIACETIN

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

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

2.2. Label elements

Regulation (EC) No 1272/2008

Special labelling of certain mixtures

EUH210 Safety data sheet available on request.

Additional advice on labelling

Label elements: none.

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

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Relevant ingredients

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
102-76-1	TRIACETIN			98,5-99 %
	203-051-9		01-2119484873-24	
227456-27-1	NATURAL-3-MERCAPTO-2-METHYL-1-PENTANOL			1-1,5 %
	607-151-7			
	Acute Tox. 4; H302			

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		
102-76-1	203-051-9	TRIACETIN	98,5-99 %
	inhalation: LC50 = >1721 mg/l (vapours); dermal: LD50 = >5000 mg/kg; oral: LD50 = >2000 mg/kg		
227456-27-1	607-151-7	NATURAL-3-MERCAPTO-2-METHYL-1-PENTANOL	1-1,5 %
	oral: ATE = 500 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. Heating causes rise in pressure with risk of bursting.

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

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6.1. Personal precautions, protective equipment and emergency procedures

General advice

Use personal protection equipment.

6.2. Environmental precautions

Do not allow uncontrolled discharge of product into the environment.

6.3. Methods and material for containment and cleaning up

For cleaning up

Ventilate affected area.

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.

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
102-76-1	TRIACETIN			
Worker DNEL, long-term		inhalation	systemic	35,275 mg/m ³
Worker DNEL, long-term		dermal	systemic	5 mg/kg bw/day
Consumer DNEL, long-term		inhalation	systemic	8,7 mg/m ³
Consumer DNEL, long-term		dermal	systemic	2,5 mg/kg bw/day
Consumer DNEL, long-term		oral	systemic	2,5 mg/kg bw/day

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PNEC values

CAS No	Name of agent	
Environmental compartment		Value
102-76-1	TRIACETIN	
Freshwater		1,88 mg/l
Freshwater (intermittent releases)		1 mg/l
Marine water		0,188 mg/l
Freshwater sediment		4,73 mg/kg
Marine sediment		0,473 mg/kg
Secondary poisoning		0,07 mg/kg
Micro-organisms in sewage treatment plants (STP)		1088 mg/l
Soil		0,57 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 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:		
Odour:	cooked, meaty, onion-like	
Melting point/freezing point:		not determined
Boiling point or initial boiling point and boiling range:		259 °C
Flammability:		not determined
Lower explosion limits:		1,1 vol. %
Upper explosion limits:		7,7 vol. %
Flash point:		>98,8 °C
Auto-ignition temperature:		not determined
Decomposition temperature:		not determined
pH-Value:		not determined
Viscosity / kinematic:		not applicable
Water solubility:	The study does not need to be conducted because the substance is known to be insoluble in water.	
Solubility in other solvents		
not determined		

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Partition coefficient n-octanol/water:	not determined
Vapour pressure: (at 20 °C)	<0,001 hPa
Density:	1,158011 g/cm ³
Relative vapour density:	not determined
Particle characteristics:	not applicable

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

The product is not: Explosive.

Oxidizing properties

The product is not: oxidising.

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.

ATEmix calculated

ATE (oral) > 5000 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
102-76-1	TRIACETIN				
	oral	LD50 >2000 mg/kg	Rat	REACH registration	OECD 401
	dermal	LD50 >5000 mg/kg	Rabbit	REACH registration	OECD 402
	inhalation (4 h) vapour	LC50 >1721 mg/l	Rat	REACH registration	OECD 403
227456-27-1	NATURAL-3-MERCAPTO-2-METHYL-1-PENTANOL				
	oral	ATE 500 mg/kg			

Irritation and corrosivity

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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.

Other information

The mixture is classified as not hazardous according to regulation (EC) No 1272/2008 [CLP].

SECTION 12: Ecological information

12.1. Toxicity

Based on available data, the classification criteria are not met.

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
102-76-1	TRIACETIN					
	Acute fish toxicity	LC50 >100 mg/l	96 h	Oryzias latipes (Ricefish)	REACH registration	OECD 203
	Acute algae toxicity	ErC50 >940 mg/l	72 h	Pseudokirchneriella subcapitata	REACH registration	OECD 201
	Acute crustacea toxicity	EC50 380 mg/l	48 h	Daphnia magna (Big water flea)	REACH registration	EU Method C.2
	Crustacea toxicity	NOEC >94 mg/l	21 d	Daphnia magna (Big water flea)	REACH registration	OECD 211

12.2. Persistence and degradability

The product has not been tested.

CAS No	Chemical name			
	Method	Value	d	Source
	Evaluation			
102-76-1	TRIACETIN			
	OECD 301 B	77-80%	26	REACH Dossier
	Readily biodegradable (according to OECD criteria).			
	OECD 301 B	69-70%	12	REACH Dossier
	Readily biodegradable (according to OECD criteria).			
	OECD 301 B	29-37%	6	REACH Dossier
	Readily biodegradable (according to OECD criteria).			

12.3. Bioaccumulative potential

The product has not been tested.

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Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
102-76-1	TRIACETIN	0,25
227456-27-1	NATURAL-3-MERCAPTO-2-METHYL-1-PENTANOL	1,626

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.

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)

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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 dangerous good in sense of this transport regulation.

14.7. Maritime transport in bulk according to IMO instruments

No dangerous good in sense of this transport regulation.

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulatory information

Directive 2010/75/EU on industrial emissions:	99 %
Directive 2004/42/EC on VOC in paints and varnishes:	1 %
Information according to Directive 2012/18/EU (SEVESO III):	Not subject to 2012/18/EU (SEVESO III)

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

Acute Tox: Acute toxicity
 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
 EC/EEC: European Community/European Economic Community
 EU: European Union
 CAS: Chemical Abstracts Service
 DNEL: Derived No Effect Level
 DMEL: Derived Minimal Effect Level
 PNEC: Predicted No Effect Concentration
 ATE: Acute toxicity estimate
 LC50: Lethal concentration, 50%
 LD50: Lethal dose, 50%
 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
 M-factor: Multiplying factor
 ADR: Accord européen sur le transport des marchandises dangereuses par Route
 (European Agreement concerning the International Carriage of Dangerous Goods by Road)
 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)
 IMDG: International Maritime Code for Dangerous Goods
 EmS: Emergency Schedules
 MFAG: Medical First Aid Guide
 IATA: International Air Transport Association
 DGR: Dangerous Goods Regulations
 ICAO: International Civil Aviation Organization
 TI: Technical Instructions
 MARPOL: International Convention for the Prevention of Marine Pollution from Ships
 IBC: Intermediate Bulk Container
 VOC: volatile organic compound
 SVHC: Substance of Very High Concern
 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.
 EUH210 Safety data sheet available on request.

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.)