

Safety Data Sheet

according to Regulation (EC) No 1907/2006

4-MERCAPTO-4-METHYL-2-PENTANONE 1% IN TRIACETIN

Revision date: 04.03.2025

Product code: 399740

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

1.1. Product identifier

4-MERCAPTO-4-METHYL-2-PENTANONE 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

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)			
102-76-1	TRIACETIN			98,5 - 99 %
	203-051-9		01-2119484873-24	
19872-52-7	NATURAL 4-MERCAPTO-4-METHYL-2-PENTANONE			1 - 1,5 %
	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	
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	

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

Observe risk of aspiration if vomiting occurs. 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

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

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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. 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	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

PNEC values

CAS No	Name of agent	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

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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:	colourless	
Melting point/freezing point:		not determined
Boiling point or initial boiling point and boiling range:		259 °C
Flammability:		not applicable
		not applicable
Lower explosion limits:		1,1 vol. %
Upper explosion limits:		7,7 vol. %
Flash point:		>100 °C
Auto-ignition temperature:		433 °C
Decomposition temperature:		not determined
pH-Value:		not determined
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	
Partition coefficient n-octanol/water:		not determined
Vapour pressure:		<0,001 hPa
(at 20 °C)		
Density:		1,16 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.

Oxidizing properties

The product is not: oxidising.

Other safety characteristics

Evaporation rate:	not determined
Solvent content:	99,00 %
Solid content:	0%

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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

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

Acute toxicity

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

11.2. Information on other hazards

Endocrine disrupting properties

No information available.

Other information

No information available.

Further information

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

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
102-76-1	TRIACETIN					
	Acute fish toxicity	LC50 mg/l	>100	96 h Oryzias latipes (Ricefish)	REACH registration	OECD 203
	Acute algae toxicity	ErC50 mg/l	>940	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.

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.

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
102-76-1	TRIACETIN	0,25
19872-52-7	NATURAL 4-MERCAPTO-4-METHYL-2-PENTANONE	1,432

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.

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

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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

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

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Directive 2004/42/EC on VOC in
paints and varnishes: 1 % (11,6 g/l)

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

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>
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)

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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.)