

safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



α + β -Thujone pure

article number: **9540**
Version: **1.0 en**

date of compilation: 2016-12-09

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

1.1 Product identifier

Identification of the substance	α+β-Thujone
Article number	9540
Registration number (REACH)	This information is not available.
EC number	none
CAS number	76231-76-0

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses: laboratory chemical

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

Telephone: +49 (0) 721 - 56 06 0

Telefax: +49 (0) 721 - 56 06 149

e-mail: sicherheit@carlroth.de

Website: www.carlroth.de

Competent person responsible for the safety data sheet : Department Health, Safety and Environment

e-mail (competent person) : sicherheit@carlroth.de

1.4 Emergency telephone number

Emergency information service **Poison Centre Munich: +49/(0)89 19240**

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
3.1O	acute toxicity (oral)	(Acute Tox. 4)	H302
3.4S	skin sensitisation	(Skin Sens. 1)	H317
4.1C	hazardous to the aquatic environment - chronic hazard	(Aquatic Chronic 3)	H412

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Remarks

For full text of Hazard- and EU Hazard-statements: see SECTION 16.

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP)

Signal word

Warning

Pictograms



Hazard statements

H302	Harmful if swallowed.
H317	May cause an allergic skin reaction.
H412	Harmful to aquatic life with long lasting effects.

Precautionary statements

Precautionary statements - prevention

P273	Avoid release to the environment.
P280	Wear protective gloves.

Precautionary statements - response

P302+P352	IF ON SKIN: Wash with plenty of soap and water.
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Labelling of packages where the contents do not exceed 125 ml

Signal word: **Warning**

Symbol(s)



H317	May cause an allergic skin reaction.
H412	Harmful to aquatic life with long lasting effects.
P280	Wear protective gloves.
P302+P352	IF ON SKIN: Wash with plenty of soap and water.

2.3 Other hazards

There is no additional information.

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SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	α + β -Thujone
CAS number	76231-76-0
Molecular formula	C ₁₀ H ₁₆ O
Molar mass	152,2 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Do not leave affected person unattended.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Wash with plenty of soap and water. In case of skin reactions, consult a physician.

Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

Following ingestion

Rinse mouth immediately and drink plenty of water. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

Irritant effects, Allergic reactions, Headache, Vertigo, Nausea, Vomiting, Diarrhoea, Spasms, Unconsciousness

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings
water spray, foam, dry extinguishing powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

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5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

In case of fire may be liberated: carbon monoxide (CO), carbon dioxide (CO₂)

5.3 Advice for firefighters

Do not allow firefighting water to enter drains or water courses. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Do not breathe vapour/spray. Avoid contact with skin and eyes.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

6.3 Methods and material for containment and cleaning up

Advices on how to contain a spill

Covering of drains.

Advices on how to clean up a spill

Absorb with liquid-binding material (e.g. sand, diatomaceous earth, acid- or universal binding agents).

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provide adequate ventilation. Avoid exposure.

• Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs. Wash hands before breaks and after work.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed. May cause decomposition by long-term light influence.

Incompatible substances or mixtures

Observe hints for combined storage.

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Consideration of other advice

- **Ventilation requirements**

Use local and general ventilation.

- **Specific designs for storage rooms or vessels**

Recommended storage temperature: 15 - 25 °C.

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

No data available. Data are not available.

8.2 Exposure controls

Individual protection measures (personal protective equipment)



Eye/face protection

Use safety goggle with side protection.

Skin protection

- **hand protection**

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. 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.

- **type of material**

NBR (Nitrile rubber)

- **material thickness**

>0,11 mm

- **breakthrough times of the glove material**

>480 minutes (permeation: level 6)

- **other protection measures**

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection

Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C , colour code: Brown).

Environmental exposure controls

Keep away from drains, surface and ground water.

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SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance

Physical state	liquid (fluid)
Colour	colourless - light yellow
Odour	characteristic
Odour threshold	No data available

Other physical and chemical parameters

pH (value)	This information is not available.
Melting point/freezing point	not determined
Initial boiling point and boiling range	200 - 202 °C
Flash point	67 °C
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)
<u>Explosive limits</u>	
• lower explosion limit (LEL)	this information is not available
• upper explosion limit (UEL)	this information is not available
Explosion limits of dust clouds	not relevant
Vapour pressure	This information is not available.
Density	0,92 - 0,93 g/cm ³
Vapour density	This information is not available.
Bulk density	Not applicable
Relative density	Information on this property is not available.
<u>Solubility(ies)</u>	
Water solubility	insoluble
<u>Partition coefficient</u>	
n-octanol/water (log KOW)	This information is not available.
Auto-ignition temperature	Information on this property is not available.
Decomposition temperature	no data available
Viscosity	not determined
Explosive properties	Shall not be classified as explosive
Oxidising properties	none

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9.2 Other information

There is no additional information.

Refractive index 1,452 - 1,454

SECTION 10: Stability and reactivity

10.1 Reactivity

In case of warming: Vapours can form explosive mixtures with air.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: Alkalis, Oxidisers, Acids

10.4 Conditions to avoid

Keep away from heat.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Exposure route	Endpoint	Value	Species	Source
oral	LD50	500 mg/kg	rat	Lit.

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

May cause an allergic skin reaction. May cause sensitization by skin contact.

Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor as a reproductive toxicant

- **Specific target organ toxicity - single exposure**

Shall not be classified as a specific target organ toxicant (single exposure).

- **Specific target organ toxicity - repeated exposure**

Shall not be classified as a specific target organ toxicant (repeated exposure).

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Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

- **If swallowed**

nausea, abdominal pain, vomiting, diarrhoea

- **If in eyes**

irritant effects

- **If inhaled**

Irritating to respiratory system, dizziness, headache, vertigo

- **If on skin**

Frequently or prolonged contact with skin may cause dermal irritation, Allergic reactions

Other information

Circulatory collapse, Cardiac arrhythmias, Spasms, Unconsciousness, Liver and kidney damage

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life with long lasting effects.

Aquatic toxicity (chronic)

May cause long-term adverse effects in the aquatic environment.

12.2 Process of degradability

Theoretical Oxygen Demand: 2,837 mg/mg
Theoretical Carbon Dioxide: 2,891 mg/mg

12.3 Bioaccumulative potential

Data are not available.

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains. Avoid release to the environment. Refer to special instructions/safety data sheets.

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13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions.

SECTION 14: Transport information

- | | | |
|------|----------------------------|--|
| 14.1 | UN number | (not subject to transport regulations) |
| 14.2 | UN proper shipping name | not relevant |
| 14.3 | Transport hazard class(es) | not relevant |
| | Class | - |
| 14.4 | Packing group | not relevant |
| 14.5 | Environmental hazards | none (non-environmentally hazardous acc. to the dangerous goods regulations) |
- 14.6 **Special precautions for user**
There is no additional information.
- 14.7 **Transport in bulk according to Annex II of MARPOL and the IBC Code**
The cargo is not intended to be carried in bulk.
- 14.8 **Information for each of the UN Model Regulations**
- **Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)**
Not subject to ADR, RID and ADN.
 - **International Maritime Dangerous Goods Code (IMDG)**
Not subject to IMDG.
 - **International Civil Aviation Organization (ICAO-IATA/DGR)**
Not subject to ICAO-IATA.

SECTION 15: Regulatory information

- 15.1 **Safety, health and environmental regulations/legislation specific for the substance or mixture**
- Relevant provisions of the European Union (EU)**
- **Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)**
Not listed.
 - **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**
Not listed.
 - **Regulation 850/2004/EC on persistent organic pollutants (POP)**
Not listed.

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- **Restrictions according to REACH, Annex XVII**

not listed

- **List of substances subject to authorisation (REACH, Annex XIV)**

not listed

- **Limitation of emissions of volatile organic compounds due to the use of organic solvents in certain paints and varnishes and vehicle refinishing products (2004/42/EC, Deco-Paint Directive)**

VOC content 100 %

- **Directive on industrial emissions (VOCs, 2010/75/EU)**

VOC content 100 %

Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II

not listed

Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

not listed

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DGR	Dangerous Goods Regulations (see IATA/DGR)
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
VOC	Volatile Organic Compounds

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Abbr.	Descriptions of used abbreviations
vPvB	very Persistent and very Bioaccumulative

Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)

List of relevant phrases (code and full text as stated in chapter 2 and 3)

Code	Text
H302	harmful if swallowed
H317	may cause an allergic skin reaction
H412	harmful to aquatic life with long lasting effects

Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.