

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## $\alpha,\beta$ -Thujone (isomers) pure

article number: **9540**  
Version: **GHS 3.0 en**  
Replaces version of: 2022-02-23  
Version: (GHS 2)

date of compilation: 2016-12-09  
Revision: 2024-03-03

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

### 1.1 Product identifier

Identification of the substance  **$\alpha,\beta$ -Thujone (isomers) pure**  
Article number 9540  
CAS number 76231-76-0

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

Relevant identified uses: Laboratory chemical  
Laboratory and analytical use  
Uses advised against: Do not use for private purposes (household).  
Food, drink and animal feedingstuffs.

### 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

| Name   | Street          | Postal code/city   | Telephone | Website |
|--|-----------------|--------------------|-----------|---------|
| NSW Poisons Information Centre<br>Childrens Hospital | Hawkesbury Road | 2145 Westmead, NSW | 131126    |         |

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

Classification acc. to GHS

| Section | Hazard class          | Category | Hazard class and category | Hazard statement |
|---------|-----------------------|----------|---------------------------|------------------|
| 2.6     | Flammable liquid      | 4        | Flam. Liq. 4              | H227             |
| 3.10    | Acute toxicity (oral) | 4        | Acute Tox. 4              | H302             |
| 3.4S    | Skin sensitisation    | 1        | Skin Sens. 1              | H317             |

For full text of abbreviations: see SECTION 16

#### The most important adverse physicochemical, human health and environmental effects

The product is combustible and can be ignited by potential ignition sources.

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### 2.2 Label elements

#### Labelling

#### Signal word

#### Warning

#### Pictograms

GHS07



#### Hazard statements

|      |                                     |
|------|-------------------------------------|
| H227 | Combustible liquid                  |
| H302 | Harmful if swallowed                |
| H317 | May cause an allergic skin reaction |

#### Precautionary statements

##### Precautionary statements - prevention

|      |   |
|------|---|
| P210 | Keep away from heat/sparks/open flames/hot surfaces. - No smoking         |
| P261 | Avoid breathing dust/fume/gas/mist/vapours/spray                          |
| P280 | Wear protective gloves/protective clothing/eye protection/face protection |

##### Precautionary statements - response

|           |   |
|-----------|---|
| P302+P352 | IF ON SKIN: Wash with plenty of soap and water                                  |
| P333+P313 | If skin irritation or rash occurs: Get medical advice/attention                 |
| P370+P378 | In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction |

##### Precautionary statements - disposal

|      |  |
|------|--|
| P501 | Dispose of contents/container to industrial combustion plant |
|------|--|

### 2.3 Other hazards

This material is combustible, but will not ignite readily.

#### Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

#### Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                   |                                   |
|-------------------|-----------------------------------|
| Name of substance | $\alpha,\beta$ -Thujone (isomers) |
| Molecular formula | $C_{10}H_{16}O$                   |
| Molar mass        | 152.2 g/mol                       |
| CAS No            | 76231-76-0                        |

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## SECTION 4: First aid measures

### 4.1 Description of first aid measures



#### General notes

Take off contaminated clothing.

#### Following inhalation

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

#### Following skin contact

After contact with skin, wash immediately with plenty of water. In case of skin reactions, consult a physician.

#### Following eye contact

Rinse cautiously with water for several minutes.

#### Following ingestion

Rinse mouth with water (only if the person is conscious). Call a doctor.

### 4.2 Most important symptoms and effects, both acute and delayed

Vomiting, Allergic reactions

### 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 firefighting measures to the fire surroundings!  
water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO<sub>2</sub>)

#### Unsuitable extinguishing media

water jet

### 5.2 Special hazards arising from the substance or mixture

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours may form explosive mixtures with air.

#### Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>)

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### 5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. 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

Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

### 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

#### Advice on how to contain a spill

Covering of drains.

#### Advice on how to clean up a spill

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

#### Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

### 6.4 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

Provision of sufficient ventilation.

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



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge.

#### Advice on general occupational hygiene

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

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

#### 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)

This information is 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. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

#### • 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.

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### 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.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

|  |  |
|--|--|
| Physical state   | liquid   |
| Colour   | colourless - light yellow                        |
| Odour  | characteristic                                   |
| Melting point/freezing point                             | not determined                                   |
| Boiling point or initial boiling point and boiling range | 200 – 202 °C                                     |
| Flammability   | flammable liquid in accordance with GHS criteria |
| Lower and upper explosion limit                          | not determined                                   |
| Flash point  | 67 °C  |
| Auto-ignition temperature                                | not determined                                   |
| Decomposition temperature                                | not relevant                                     |
| pH (value)   | not determined                                   |
| Kinematic viscosity                                      | not determined                                   |
| <u>Solubility(ies)</u>                                   |  |
| Water solubility   | not determined                                   |
| <u>Partition coefficient</u>                             |  |
| Partition coefficient n-octanol/water (log value):       | this information is not available                |
| Vapour pressure  | not determined                                   |
| <u>Density and/or relative density</u>                   |  |
| Density  | 0.92 – 0.93 g/cm <sup>3</sup>                    |
| Relative vapour density                                  | Information on this property is not available.   |
| Particle characteristics                                 | not relevant (liquid)                            |

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### Other safety parameters

Oxidising properties none

### 9.2 Other information

Information with regard to physical hazard classes: There is no additional information.

Other safety characteristics:

Refractive index 1.452 - 1.454

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

It's a reactive substance. Risk of ignition.

#### If heated

Risk of ignition. Vapours may 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:** strong oxidiser

### 10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

### 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

**Classification acc. to GHS**

#### Acute toxicity

Harmful if swallowed.

| Acute toxicity |          |           |         |        |        |
|----------------|----------|-----------|---------|--------|--------|
| Exposure route | Endpoint | Value     | Species | Method | 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.

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### **Respiratory or skin sensitisation**

May cause an allergic skin reaction.

### **Germ cell mutagenicity**

Shall not be classified as germ cell mutagenic.

### **Carcinogenicity**

Shall not be classified as carcinogenic.

### **Reproductive toxicity**

Shall not be classified 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).

### **Aspiration hazard**

Shall not be classified as presenting an aspiration hazard.

### **Symptoms related to the physical, chemical and toxicological characteristics**

#### • **If swallowed**

Data are not available.

#### • **If in eyes**

Data are not available.

#### • **If inhaled**

Data are not available.

#### • **If on skin**

May produce an allergic reaction, pruritis, localised redness

#### • **Other information**

none

### **11.2 Endocrine disrupting properties**

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

## **SECTION 12: Ecological information**

### **12.1 Toxicity**

Harmful to aquatic life with long lasting effects.

### **12.2 Persistence and degradability**

Theoretical Oxygen Demand:  $2.837 \text{ mg/mg}$   
Theoretical Carbon Dioxide:  $2.891 \text{ mg/mg}$

### **12.3 Bioaccumulative potential**

Data are not available.

### **12.4 Mobility in soil**

Data are not available.



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### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

### 12.7 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.

#### Waste treatment of containers/packagings

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

### 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. Non-contaminated packages may be recycled.

## SECTION 14: Transport information

- |      |  |  |
|------|--|--|
| 14.1 | <b>UN number</b>   | not subject to transport regulations   |
| 14.2 | <b>UN proper shipping name</b>                                 | not assigned   |
| 14.3 | <b>Transport hazard class(es)</b>                              | not assigned   |
| 14.4 | <b>Packing group</b>   | not assigned   |
| 14.5 | <b>Environmental hazards</b>                                   | non-environmentally hazardous acc. to the dangerous goods regulations              |
| 14.6 | <b>Special precautions for user</b>                            | There is no additional information.  |
| 14.7 | <b>Transport in bulk according to IMO instruments</b>          | The cargo is not intended to be carried in bulk.                                   |
| 14.8 | <b><u>Information for each of the UN Model Regulations</u></b> |  |
|      | <b>Transport information</b>                                   | <b>National regulations</b>  |
|      |  | <b>Additional information(UN RTDG)</b>   |
|      |  | Not subject to transport regulations. UN RTDG                                      |
|      |  | <b>International Maritime Dangerous Goods Code (IMDG) - Additional information</b> |
|      |  | Not subject to IMDG.   |

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### International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Not subject to ICAO-IATA.

## SECTION 15: Regulatory information

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

There is no additional information.

#### Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

#### National inventories

| Country | Inventory | Status              |
|---------|-----------|---------------------|
| VN      | NCI       | substance is listed |

#### Legend

NCI National Chemical Inventory

### 15.2 Chemical Safety Assessment

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

## SECTION 16: Other information

### Indication of changes (revised safety data sheet)

| Section | Former entry (text/value) | Actual entry (text/value)   | Safety-relevant |
|---------|---------------------------|---|-----------------|
| 2.3     |                           | Endocrine disrupting properties:<br>Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$ . | yes             |
| 15.1    |                           | National inventories  | yes             |
| 15.1    |                           | National inventories:<br>change in the listing (table)  | yes             |

### Abbreviations and acronyms

| Abbr.    | Descriptions of used abbreviations   |
|----------|--|
| CAS      | Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)                           |
| DGR      | Dangerous Goods Regulations (see IATA/DGR)   |
| ED       | Endocrine disruptor  |
| 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  |
| LD50     | Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval |

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| Abbr.   | Descriptions of used abbreviations                    |
|---------|---|
| PBT     | Persistent, Bioaccumulative and Toxic                 |
| UN RTDG | UN Recommendations on the Transport of Dangerous Good |
| vPvB    | Very Persistent and very Bioaccumulative              |

### Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

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

| Code | Text                                 |
|------|--------------------------------------|
| H227 | Combustible liquid.                  |
| H302 | Harmful if swallowed.                |
| H317 | May cause an allergic skin reaction. |

### Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.