

Your contact at PhytoLab:
Reference Substances
Tel.: +49 9163 88-395
ref-substances@phytolab.de
<https://phyproof.phytolab.com>

Certificate of analysis

Article:	89286 (-)- α -Thujone
Material batch:	1001944
Sample-ID:	269323
End of analysis:	07/2025
Expiry date:	03/2029

Test	Unit	Specified value	Testresult
Appearance, SOP 100005		liquid	conform
Color, SOP 100006		colorless	conform
Identity test (1H-NMR-spectroscopy), (outsourced), SOP 206010		conform	conform
Identity test (13C-NMR-spectroscopy), (outsourced), SOP 206020		conform	conform
Identity test (GC-MS,EI), SOP 204160		conform	conform
Identity test (IR-spectroscopy), Ph. Eur. 2.2.24, Absorption Spectrophotometry, Infrared (01/2021:20224) and USP chapter <197>, Spectroscopic Identification Tests (Official as of 01-Sep-2021), SOP 206000		conform	conform
Determination of water (coulometric titration), Ph. Eur. 2.5.32, Water: micro determination (07/2019:20532), SOP 304291, Vers. 2018-01 (double analysis) Mean value	%		0.2
Specific optical rotation, Ph. Eur. 2.2.7, Optical rotation (07/2018:20207), SOP 305501 (c = 0.50; EtOH)			-14.72

Certificate of analysis

Article: 89286 (-)- α -Thujone
 Material batch: 1001944

Test	Unit	Specified value	Testresult
Alpha-Thujone (GC), method 2 (% AU), SOP 400398	%	≥ 90.00	95.93
Inorganic impurities, (ICP-MS), for reference substances, SOP 811701:	%		<0.1
Calcium			
Potassium	%		<0.1
Magnesium	%		<0.1
Sulfur	%		<1.0
Sodium	%		<0.1
Phosphorus	%		<0.1
Aluminium	%		<0.1
Determination of residual solvent residues (head-space-GC-FID), SOP 805765	%		
Residual solvent content (LOQ: 0.050)			0.094
Content, SOP 890000, calculated in (%): $(100 - \text{water} - \text{residual solvents} - \text{inorganic impurities}) \times \text{chromatographic purity} / 100$	%		96

This PhytoLab phyproof© reference standard is by definition a primary reference standard and does not need to be qualified against any other reference standard. The identity of the reference standard has been substantiated by at least two independent analytical methods such as IR, NMR, UV or MS analysis. A mass balance approach, which takes chromatographic purity into account, as well as the contents of water, residual solvents, inorganic impurities, and the counter ion (if the reference standard is present as a salt) is applied in the calculation of the absolute purity as given in this COA (see description of SOP 8900XX).

The absolute purity value (and not just the chromatographic purity result obtained by

Certificate of analysis

Article: 89286 (-)- α -Thujone
Material batch: 1001944

means of HPLC or GC) must be used in all quantitative calculations as the chromatographic techniques do not yet account for water, residual solvents and inorganic impurities.

Vestenbergsreuth, 18/Jul/2025

Sibylle Friess

QC Reference Substances

This is a computer print and valid without signature. A signed certificate of analysis can be taken on request.

Certificate of analysis

Article: 89286 (-)- α -Thujone
Material batch: 1001944

Further information:

Shelf life/stability: The stated expiry date applies when the reference substance is stored in the original unopened container within the specified temperature range. PhytoLab does not guarantee the stability of the reference substance once the vial has been opened.

Long-term storage and handling: The reference standard should be stored in the original unopened vial, protected against light and humidity in an airtight container, within the temperature range given on the label and accompanying data sheet. If stored below room temperature, the vial should be warmed up to room temperature in a desiccator before it is opened in order to avoid condensation of humidity. The user assumes responsibility for deciding how previously opened reference standard vials should be used and the user must ensure that the contents of opened vials are still suitable for their intended use.

Exact weight: the exact weight of each vial is given on the label of the inner vial to two decimal places. This information may be used to produce stock solutions of a known concentration without having to weigh in the reference substance again. If used for this purpose, the content of the vial must be quantitatively transferred to a volumetric flask and filled up to the required level. Please note that PhytoLab is unable to guarantee the stability of the reference standard in solution.

Intended use: this reference standard is solely intended for laboratory analytical purposes, research & development, and scientific teaching and training purposes. It may not be used for any other purpose and particularly not for use in, or the production of, food, animal feed, human or veterinary drugs, cosmetics, medicinal products or diagnostic agents, including in-vitro diagnostic agents. PhytoLab is unable to guarantee the suitability of this reference standard for any particular application other than its qualitative and quantitative use in chromatography and identification testing.

Further information about this reference standard can be found on the accompanying data sheet or in our webshop. Spectral and chromatographic data, and a description of the applied chromatographic method, are provided in the attachments to this COA. A detailed explanation of all data given on the COA can be found in the guide that is available from the download area in our webshop, where you can also download all of the safety data sheets.