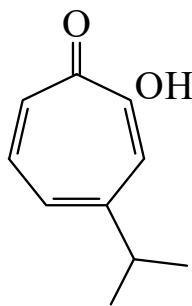




>>Entry Name: 2-Hydroxy-4(6)-isopropyl-2,4,6-cycloheptatrien-1-one

Synonym(s): 2-Hydroxy-4(6)-(1-methylethyl)-2,4,6-cycloheptatrien-1-one, 9Cl. 4(6)-Isopropyltropolone. β -Thujaplicin. Hinokitiol



CAS Registry Number: 499-44-5

Molecular Formula: C₁₀H₁₂O₂

Molecular Weight: 164.204

Accurate Mass: 164.08373

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Biological Source: Occurs in *Juniperus conferta*, *Juniperus chinensis*, *Juniperus communis*, *Juniperus thurifera*, *Juniperus utahensis*, in the oil of the wood of the Hinoki tree (*Chamaecyparis obtusa*) and in the heartwood of *Thuja plicata*, *Thuja occidentalis*. Widespread in the Cupressaceae

Use/Importance: Antifungal substance. Also shows strong insecticidal and plant growth inhibitory props.

Physical Description: Cryst. (petrol)

Melting Point: Mp 52-52.5°

pKa Value: pK_{a1} 6.72 (25°, I 2.0)

Hazard & Toxicity: LD₅₀ (mus, ipr) 85 mg/kg

Aldrich: 46952-1

>>Derivative: Cu complex

Melting Point: Mp 177°

>>Derivative: 1-O- β -D-Glucopyranoside

Synonym(s): Cupressotropolone A

Molecular Formula: C₁₆H₂₂O₇

Molecular Weight: 326.346

Accurate Mass: 326.136555

Percentage Composition: C 58.89%; H 6.79%; O 34.32%

Biological Source: Constit. of *Cupressus sempervirens*

Use/Importance: Shows antifungal props.

UV: [neutral] $\lambda_{\max}$ 240 (); 330 () (MeOH) (Berdy)

Other Data: Derived from the 2-oxo tautomer

References:

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