



Physical Description: Oil

Boiling Point: Bp₃₂ 54-56°

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 3000 mg/kg

Aldrich: W50460-2

>> **Derivative:** 3,5-Dinitrobenzoyl

Melting Point: Mp 71°

>> **Derivative:** 3,4-Dihydroxy-*E*-cinnamoyl

Synonym(s): 3-Methyl-2-butenyl caffeate

CAS Registry Number: 118971-61-2

Molecular Formula: C₁₄H₁₆O₄

Molecular Weight: 248.278

Accurate Mass: 248.10486

Percentage Composition: C 67.73%; H 6.50%; O 25.78%

Biological Source: Constit. of *Populus* spp. and propolis

Biological Use/Importance: Antiviral agent and allergenic

>> **Derivative:** 3,4-Dihydroxy-*Z*-cinnamoyl

CAS Registry Number: 119644-11-0

Molecular Formula: C₁₄H₁₆O₄

Molecular Weight: 248.278

Accurate Mass: 248.10486

Percentage Composition: C 67.73%; H 6.50%; O 25.78%

Biological Source: Constit. of *Populus* spp.

>> **Derivative:** 4-Hydroxy-3-methoxy-*E*-cinnamoyl

CAS Registry Number: 123022-25-3

Molecular Formula: C₁₅H₁₈O₄

Molecular Weight: 262.305

Accurate Mass: 262.12051

Percentage Composition: C 68.69%; H 6.92%; O 24.40%

Biological Source: Constit. of *Populus violascens*

>> **Derivative:** Me ether

Synonym(s): 1-Methoxy-3-methyl-2-butene

CAS Registry Number: 22093-99-8

Molecular Formula: C₆H₁₂O

Molecular Weight: 100.16

Accurate Mass: 100.088815

Percentage Composition: C 71.95%; H 12.08%; O 15.97%

Physical Description: Liq.

Boiling Point: Bp 102-104°

References: