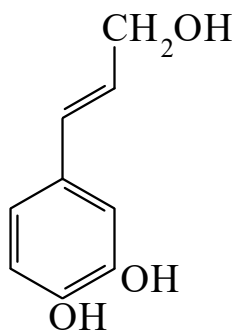




>>Entry Name: **3-(3,4-Dihydroxyphenyl)-2-propen-1-ol**

Synonym(s): 4-(3-Hydroxy-1-propenyl)-1,2-benzenediol, 9CI. Caffeyl alcohol. 3,4-Dihydroxycinnamyl alcohol



CAS Registry Number: 3598-26-3

Related CAS Registry Numbers(s): 18604-50-7 77355-78-3 81532-11-8 113349-27-2 115330-92-2 125164-73-0

Molecular Formula: C₉H₁₀O₃

Molecular Weight: 166.176

Accurate Mass: 166.062995

Percentage Composition: C 65.05%; H 6.07%; O 28.88%

General Statement: (*E*)-config. assumed for derivs. except where (*Z*)-config. is certain

>>Variant: (*E*)-form

Molecular Formula: C₉H₁₀O₃

Molecular Weight: 166.176

Accurate Mass: 166.062995

Percentage Composition: C 65.05%; H 6.07%; O 28.88%

Melting Point: Mp 144-145°

>>Derivative: 3'-Me ether

Synonym(s): 3-(4-Hydroxy-3-methoxyphenyl)-2-propen-1-ol. 4-(3-Hydroxy-1-propenyl)-2-methoxyphenol, 9CI. **Coniferyl alcohol**. Lubanol

CAS Registry Number: 32811-40-8

Extra CAS Registry Numbers(s): 458-35-5

Type of Compound Code(s): VG0060

Molecular Formula: C₁₀H₁₂O₃

Molecular Weight: 180.203

Accurate Mass: 180.078645

Percentage Composition: C 66.65%; H 6.71%; O 26.64%

Biological Source: Lignin degradn. substance found in sulfite liquor and in Siam benzoin gum

Physical Description: Prisms

Melting Point: Mp 78° (74-75°)

Boiling Point: Bp₃ 163-165°

Solubility: Spar. sol. hot H₂O; BERDY SOL: Sol. bases, Et₂O; fairly sol. MeOH, EtOH; poorly sol. H₂O

pKa Value: p*K*_{a1} 9.54 (25°)

Other Data: Resinified by acids

Aldrich: 22373-5

Fluka: 27740

Sigma: C9548

>>Derivative: 3'-Me ether, 1-*O*-β-D-glucopyranoside

Synonym(s): **Citrusin D**. Isoconiferin

CAS Registry Number: 65995-51-9

Type of Compound Code(s): VG0060

Molecular Formula: C₁₆H₂₂O₈

Molecular Weight: 342.345

Accurate Mass: 342.13147

Percentage Composition: C 56.14%; H 6.48%; O 37.39%

Biological Source: Isol. from *Citrus limon*, *Citrus unshiu*, *Fortunella japonica* and *Pinus sylvestris*

Biological Use/Importance: Shows antihypertensive props.

Optical Rotation: [α]_D²⁰ -16.9 (c, 4.1 in MeOH)

UV: [neutral] $\lambda_{\max}$ 275 (ϵ 5000) (MeOH)