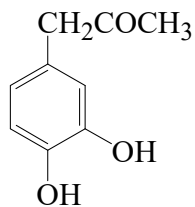




>>Entry Name: 1-(3,4-Dihydroxyphenyl)-2-propanone

Synonym(s): 3,4-Dihydroxyphenylacetone



CAS Registry Number: 2503-44-8

Type of Compound Code(s): WG4500 WI8000 WA2800

Molecular Formula: C₉H₁₀O₃

Molecular Weight: 166.176

Accurate Mass: 166.062995

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

Biological Source: Isol. from *Chrysanthemum morifolium*

Use/Importance: A component of tobacco and wood smokes, present in smoked meats. Metabolite of 2-Amino-3-(3,4-dihydroxyphenyl)-2-methylpropanoic acid [BDS26-B](#) and *N*, α -Dimethyl-3,4-(methylenedioxy)phenethylamine [NCZ31-D](#)

>>Derivative: 3'-Me ether

Synonym(s): 1-(4-Hydroxy-3-methoxyphenyl)-2-propanone, 9Cl. Guaiacylacetone. Methyl vanillyl ketone

CAS Registry Number: 2503-46-0

Molecular Formula: C₁₀H₁₂O₃

Molecular Weight: 180.203

Accurate Mass: 180.078645

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

Source/Synthesis: Hibbert ketone obt. by ethanolysis of coniferous lignin

Physical Description: Oil

Boiling Point: Bp₄ 155°. Bp_{0.2} 115°

Aldrich: 41065-9

>>Derivative: 3'-Me ether, 2,4-dinitrophenylhydrazone

Physical Description: Orange needles (EtOH)

Melting Point: Mp 125°

>>Derivative: Di-Me ether

Synonym(s): 1-(3,4-Dimethoxyphenyl)-2-propanone

CAS Registry Number: 776-99-8

Molecular Formula: C₁₁H₁₄O₃

Molecular Weight: 194.23

Accurate Mass: 194.094295

Percentage Composition: C 68.02%; H 7.26%; O 24.71%

Physical Description: Yellow oil

Boiling Point: Bp_{0.15} 93°

Refractive Index: n_D²⁰ 1.5358

Aldrich: 14121-6

>>Derivative: 5'-Methoxy, 3'-Me ether

Synonym(s): 1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-propanone. **Syringylacetone**

CAS Registry Number: 19037-58-2

Molecular Formula: C₁₁H₁₄O₄

Molecular Weight: 210.229

Accurate Mass: 210.08921

Percentage Composition: C 62.85%; H 6.71%; O 30.44%

Source/Synthesis: Hibbert ketone obt. by ethanolysis of lignin

Other Data: Not to be confused with syringalacetones A and B

References: