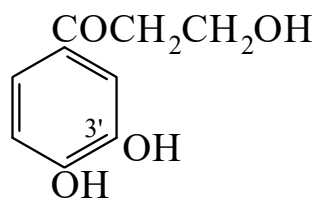




>>Entry Name: 1-(3,4-Dihydroxyphenyl)-3-hydroxy-1-propanone

Synonym(s): 3,3',4'-Trihydroxypropioiphenone. 2-(3,4-Dihydroxybenzoyl)ethanol



Molecular Formula: C₉H₁₀O₄

Molecular Weight: 182.176

Accurate Mass: 182.05791

Percentage Composition: C 59.34%; H 5.53%; O 35.13%

>>Derivative: 3'-Me ether

Synonym(s): 3-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-1-propanone, 9Cl. 3,4'-Dihydroxy-3'-methoxypropioiphenone, 8Cl. ω-Hydroxypropioiguaiacone. β-Hydroxypropiovanillone

CAS Registry Number: 2196-18-1

Type of Compound Code(s): VG0060

Molecular Formula: C₁₀H₁₂O₄

Molecular Weight: 196.202

Accurate Mass: 196.07356

Percentage Composition: C 61.22%; H 6.16%; O 32.62%

Biological Source: Isol. from *Bauhinia manca*, *Epichloe typhina*, *Leptactinia senegambica*, *Pinus armandii* and *Pinus sylvestris*. Metab. of *Pseudomonas acidovorans*

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 109-110°

>>Derivative: 3'-Me ether, di-Ac

Molecular Formula: C₁₄H₁₆O₆

Molecular Weight: 280.277

Accurate Mass: 280.09469

Percentage Composition: C 60.00%; H 5.75%; O 34.25%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 62°

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

CAS Registry Number: 114226-07-2

Type of Compound Code(s): VG0060

Molecular Formula: C₁₆H₂₂O₉

Molecular Weight: 358.344

Accurate Mass: 358.126385

Percentage Composition: C 53.63%; H 6.19%; O 40.18%

Biological Source: Isol. from *Pseudomonas sylvestris* and *Picea abies*

Optical Rotation: [α]_D²⁰ -9.5 (c, 1 in MeOH)

>>Derivative: 3-Et, 3'-Me ether

Synonym(s): 3-Ethoxy-1-(4-hydroxy-3-methoxyphenyl)-1-propanone

Type of Compound Code(s): VG0035 VG0060

Molecular Formula: C₁₂H₁₆O₄

Molecular Weight: 224.256

Accurate Mass: 224.10486

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Biological Source: Constit. of *Diospyros maritima*

Melting Point: Mp 72-74°

UV: [neutral] λ_{max} 230 (log ε 4.17); 277 (log ε 4.11); 303 (log ε 3.94) (MeOH)

References:

- Baker, S.B. *et al.*, *J.A.C.S.*, 1948, **70**, 60, (*synth*)
Kovacik, V. *et al.*, *Chem. Ber.*, 1969, **102**, 1513, (*ms*)
Andersson, R. *et al.*, *Phytochemistry*, 1988, **27**, 559, (*glucoside*)
Achenbach, H. *et al.*, *Phytochemistry*, 1988, **27**, 1835, (*isol*)
Lin, R.C. *et al.*, *Planta Med.*, 1994, **60**, 168, (*isol, uv, pmr*)
Pan, H. *et al.*, *Phytochemistry*, 1995, **39**, 1423
Kuo, Y.-H. *et al.*, *Phytochemistry*, 1998, **49**, 2505-2507, (*3-Et-3'-Me ether*)