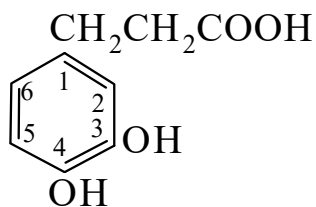




>>Entry Name: 3-(3,4-Dihydroxyphenyl)propanoic acid

ENTRY UNDER REVIEW

Synonym(s): 3,4-Dihydroxybenzenepropanoic acid, 9CI. 3,4-Dihydroxyhydrocinnamic acid, 8CI. Hydrocaffeic acid



CAS Registry Number: 1078-61-1

Type of Compound Code(s): VG0060

Molecular Formula: C₉H₁₀O₄

Molecular Weight: 182.176

Accurate Mass: 182.05791

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

Biological Source: Occurs in spores of *Lycopodium clavatum* and also in higher plants. Some occurrence in complex natural products eg. Tarchonanthuslactone [GNC75-I](#), Lycognidine [GPC91-Y](#)

Physical Description: Leaflets (H₂O)

Melting Point: Mp 139°

pKa Value: pK_{a1} 4.56; pK_{a2} 9.36; pK_{a3} 11.6 (30°, 0.1M NaClO₄)

Aldrich: 10260-1

Fluka: 54130

Sigma: H2388

>>Derivative: Et ester

CAS Registry Number: 3967-57-5

Molecular Formula: C₁₁H₁₄O₄

Molecular Weight: 210.229

Accurate Mass: 210.08921

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

Melting Point: Mp 50-52°

Aldrich: 28331-2

>>Derivative: 4-Methylpentyl ester

Type of Compound Code(s): VG0060

Molecular Formula: C₁₅H₂₂O₄

Molecular Weight: 266.336

Accurate Mass: 266.15181

Percentage Composition: C 67.65%; H 8.33%; O 24.03%

Biological Source: Constit. of *Cheirolophus mauritanicus*

Physical Description: Gum

>>Derivative: 4-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside], Me ester

Synonym(s): Citrusin F

CAS Registry Number: 134860-04-1

Type of Compound Code(s): WI2000 VG0060

Molecular Formula: C₂₂H₃₂O₁₄

Molecular Weight: 520.486

Accurate Mass: 520.17921

Percentage Composition: C 50.77%; H 6.20%; O 43.04%

Biological Source: Isol. from lemon peel oil (*Citrus limon*)

Physical Description: Oil

Optical Rotation: [α]_D²² -4.68 (c, 0.1 in MeOH)