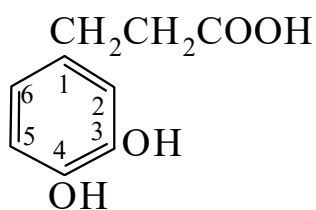




>>Entry Name: 3-(3,4-Dihydroxyphenyl)propanoic acid

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: $\text{C}_9\text{H}_{10}\text{O}_4$

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 (H_2O)

Melting Point: Mp 139°

pKa Value: $\text{p}K_{\text{a}1}$ 4.56; $\text{p}K_{\text{a}2}$ 9.36; $\text{p}K_{\text{a}3}$ 11.6 (30°, 0.1M NaClO_4)

Aldrich: 10260-1

Fluka: 54130

Sigma: H2388

>>Derivative: Et ester

CAS Registry Number: 3967-57-5

Molecular Formula: $\text{C}_{11}\text{H}_{14}\text{O}_4$

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: $\text{C}_{15}\text{H}_{22}\text{O}_4$

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 $\rightarrow$ 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: $\text{C}_{22}\text{H}_{32}\text{O}_{14}$

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: $[\alpha]_{\text{D}}^{22}$ -4.68 (c, 0.1 in MeOH)