



>>Entry Name: 3-(3,5-Dihydroxyphenyl)propanoic acid

Synonym(s): 3,5-Dihydroxybenzenepropanoic acid, 9CI. 3,5-Dihydroxyhydrocinnamic acid, 8CI

CAS Registry Number: 26539-01-5

Structure by analogy with 3-(2,4-Dihydroxyphenyl)propanoic acid, [DZN30-T](#)

Molecular Formula: C₉H₁₀O₄

Molecular Weight: 182.176

Accurate Mass: 182.05791

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

Source/Synthesis: Metab. of Sinapic acid [HJX78-V](#) in rats

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 145-146°

>>Derivative: 3-Me ether

Synonym(s): 3-Hydroxy-5-methoxybenzenepropanoic acid

Molecular Formula: C₁₀H₁₂O₄

Molecular Weight: 196.202

Accurate Mass: 196.07356

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

Physical Description: Plates (H₂O)

Melting Point: Mp 127°

>>Derivative: Di-Me ether

Synonym(s): 3,5-Dimethoxybenzenepropanoic acid

CAS Registry Number: 717-94-2

Molecular Formula: C₁₁H₁₄O₄

Molecular Weight: 210.229

Accurate Mass: 210.08921

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

Physical Description: Needles (C₆H₆/petrol)

Melting Point: Mp 61-62°

>>Derivative: Di-Me ether, amide

Molecular Formula: C₁₁H₁₅NO₃

Molecular Weight: 209.244

Accurate Mass: 209.105194

Percentage Composition: C 63.14%; H 7.23%; N 6.69%; O 22.94%

Physical Description: Needles (C₆H₆/petrol)

Melting Point: Mp 80-81°

References:

Salway, A.H., *J.C.S.*, 1910, **97**, 2413

Griffiths, L.A., *Experientia*, 1970, **26**, 723

Zhao, H. *et al.*, *J. Med. Chem.*, 1997, **40**, 1186-1194, (*synth, di-Me ether, pmr, ir*)