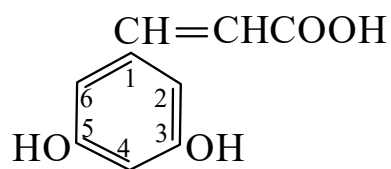




>>Entry Name: 3-(3,5-Dihydroxyphenyl)-2-propenoic acid, 9CI

Synonym(s): 3,5-Dihydroxycinnamic acid, 8CI



CAS Registry Number: 28374-93-8

Type of Compound Code(s): VG0060

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

Biological Source: Isol. from peach buds

Use/Importance: Plant growth inhibitor

Physical Description: Needles (H₂O)

Melting Point: Mp 245-246°

>>Derivative: 3-Me ether, 5-O-β-D-glucopyranoside, Me ester

Synonym(s): Linusitamarin

Type of Compound Code(s): VG0060

Molecular Formula: C₁₇H₂₂O₉

Molecular Weight: 370.355

Accurate Mass: 370.126385

Percentage Composition: C 55.13%; H 5.99%; O 38.88%

Biological Source: Constit. of *Linum usitatissimum*

Physical Description: Amorph. powder

>>Derivative: Di-Me ether

Synonym(s): 3,5-Dimethoxycinnamic acid

CAS Registry Number: 16909-11-8

Molecular Formula: C₁₁H₁₂O₄

Molecular Weight: 208.213

Accurate Mass: 208.07356

Percentage Composition: C 63.45%; H 5.81%; O 30.74%

Physical Description: Needles (H₂O)

Melting Point: Mp 175-176°

pK_a Value: pK_{a1} 4.36 (25°)

Aldrich: D13400-7

>>Derivative: Di-Me ether, pyrrolidide

Synonym(s): N-(3,5-Dimethoxycinnamoyl)pyrrolidine. 3,5-Dimethoxycinnamic acid pyrrolidide

CAS Registry Number: 102934-29-2

Type of Compound Code(s): VX0300 VX2020

Molecular Formula: C₁₅H₁₉NO₃

Molecular Weight: 261.32

Accurate Mass: 261.136494

Percentage Composition: C 68.94%; H 7.33%; N 5.36%; O 18.37%

Biological Source: Alkaloid from *Piper amalago*

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 184A, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1057B, (*nmr*)

Mauthner, F., *J. Prakt. Chem.*, 1925, **110**, 126, (*synth*)

Altree-Williams, S. *et al.*, *Aust. J. Plant Physiol.*, 1975, **2**, 105; *CA*, **83**, 40204, (*isol*)

Mukherjee, J. *et al.*, *Indian J. Chem.*, 1975, **13**, 859, (*deriv*)

Achenbach, H. *et al.*, *Planta Med.*, 1986, **52**, 12-18, (*pyrrolidide*)

Luyengi, L. *et al.*, *J. Nat. Prod.*, 1993, **56**, 2012, (*Linusitamarin*)