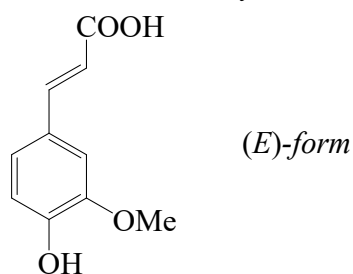




>>Entry Name: 3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid, 9CI

Synonym(s): 4-Hydroxy-3-methoxycinnamic acid, 8CI. **Ferulic acid.** Caffeic acid 3-methyl ether



CAS Registry Number: 1135-24-6

Related CAS Registry Numbers(s): 115374-26-0

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Calculated Log P Data: Log P 1.27 (calc)

Fluka: 46280

Rare Chemicals Library: S14949-7

Sigma: F3500

>>Variant: (E)-form

CAS Registry Number: 537-98-4

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Biological Source: Widely distributed in plants, first isol. from *Ferula foetida*. Metab. of a *Penicillium* sp. Found. by Bate-Smith in 33% of investigated dicotyledonous and 67% of monocotyledonous spp. Obtainable by microbial degradn. of agricultural waste, e.g wheat bran

Use/Importance: Antioxidant used in the food industry to inhibit oxidn. of fats, pastry products, etc. Antifungal agent used to prevent fruit spoilage. Investigated as starting material for microbial conversion to vanillin

Biological Use/Importance: Shows antineoplastic props. Shows cytostatic activity

Physical Description: Orthorhombic needles (H₂O)

Melting Point: Mp 174°

Solubility: BERDY SOL: Sol. MeOH, EtOAc; fairly sol. H₂O, Et₂O; poorly sol. C₆H₆, hexane

UV: [neutral] λ_{max} 236 (); 322 () (EtOH) (Berdy)

Other Data: Undergoes SOCl₂-activated polycondensation

Hazard & Toxicity: Exp. reprod. effects

Aldrich: 12870-8

>>Derivative: [β-D-Xylopyranosyl-(1→6)-β-D-glucopyranosyl] ester

CAS Registry Number: 143205-76-9

Molecular Formula: C₂₁H₂₈O₁₃

Molecular Weight: 488.444

Accurate Mass: 488.152995

Percentage Composition: C 51.64%; H 5.78%; O 42.58%

Biological Source: Constit. of the roots of *Asiasarum sieboldii*

Physical Description: Powder

Optical Rotation: [α]_D²⁴ -22 (c, 0.21 in MeOH)

>>Derivative: [α-L-Arabinofuranosyl-(1→3)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranosyl] ester

Molecular Formula: C₂₇H₃₈O₁₈

Molecular Weight: 650.586

Accurate Mass: 650.20582

Percentage Composition: C 49.85%; H 5.89%; O 44.27%

Biological Source: Constit. of soybean molasses (*Glycine* sp.)

Physical Description: Amorph. powder