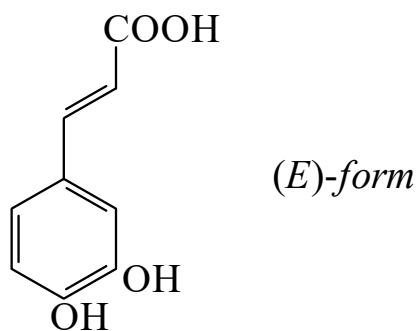




>>Entry Name: 3-(3,4-Dihydroxyphenyl)-2-propenoic acid, 9CI

Synonym(s): 3,4-Dihydroxycinnamic acid, 8CI. Caffeic acid



CAS Registry Number: 331-39-5

Extra CAS Registry Numbers(s): 2316-26-9

Type of Compound Code(s): XA1625 XA1980 XA2400 XA1950 XA3100

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

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

Use/Importance: Antioxidant

Biological Use/Importance: Antineoplastic agent. Shows anti-HIV, choleric and hepatotropic activity.

Solubility: BERDY SOL: Sol. MeOH, EtOAc; fairly sol. H₂O; poorly sol. CHCl₃, hexane

Calculated Log P Data: Log P 0.82 (calc)

UV: [acid] λ_{max} 217 (ε 20100); 300 (ε 20700); 332 (ε 24500) (as Me ester) (Derep) [base] λ_{max} (solvent not reported) (Derep) [neutral] λ_{max} 219 (ε 14700); 235 (ε 10100); 244 (ε 10500); 300 (ε 13500); 329 (ε 17100) (EtOH) (Derep) [neutral] λ_{max} 235 (); 290 (); 320 () (MeOH) (Berdy)

Aldrich: D11080-9

Fluka: 60020

Sigma: C0625

>>Variant: (E)-form

CAS Registry Number: 501-16-6

Type of Compound Code(s): XA2400 WI4400 VG0060 WA2800 WI4000 WI1000 PA2000 WI3500

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

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

Biological Source: Widespread in plants, free and as glycosides. present in fruits, cereals, wine and coffee in free and conjugated forms. Found by Bate-Smith in 66% of investigated dicotyledonous and 50% of investigated monocotyledonous plant spp.

Use/Importance: Used for spot detn. of Fe

Physical Description: Yellow cryst.

Melting Point: Mp 223-225 dec.°

pKa Value: pK_{a2} 9.07 (25°)

Calculated Log P Data: Log P 0.82 (calc)

Other Data: Forms a monohydrate. Pharmacol. active isomer

Hazard & Toxicity: Mod. allergen

>>Derivative: Me ester

CAS Registry Number: 67667-67-8

Extra CAS Registry Numbers(s): 3843-74-1

Type of Compound Code(s): VG0060

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

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

Biological Source: Isol. from plants

Physical Description: Light yellow needles (EtOH aq.)

Melting Point: Mp 158-160°

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

UV: [neutral] λ_{max} 217 (ε 15500); 242 (ε 11900); 326 (ε 18900) (MeOH) (Berdy)