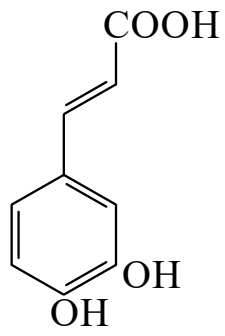
>>**Entry Name: 3-(3,4-Dihydroxyphenyl)-2-propenoic acid,** 9CI
Synonym(s): 3,4-Dihydroxycinnamic acid, 8CI. **Caffeic acid**



(*E*)-*form*

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: $C_9H_8O_4$
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, choleretic and hepatotropic activity.
Solubility: BERDY SOL: Sol. MeOH, EtOAc; fairly sol. H_2O; poorly sol. $CHCl_3$, 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: $C_9H_8O_4$
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 conjugaled 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: $C_{10}H_{10}O_4$
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, C_6H_6; poorly sol. H_2O, hexane
UV: [neutral] λ_{max} 217 (ε 15500); 242 (ε 11900); 326 (ε 18900) (MeOH) (Berdy)