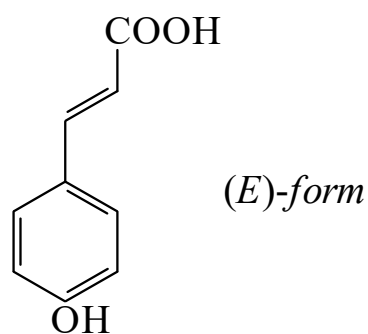




>>Entry Name: 3-(4-Hydroxyphenyl)-2-propenoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): *p*-Hydroxycinnamic acid, 8CI. *p*-Hydroxyphenylacrylic acid. ***p*-Coumaric acid**. Naringenic acid. Naringeninic acid. *p*-Cumaric acid



CAS Registry Number: 7400-08-0

Related CAS Registry Numbers(s): 830-09-1 1929-30-2 2979-06-8 3943-97-3 7139-64-2 13080-39-2 14364-05-7 117405-48-8 117405-49-9 155339-66-5 155339-67-6

Molecular Formula: C₉H₈O₃

Molecular Weight: 164.16

Accurate Mass: 164.047345

Percentage Composition: C 65.85%; H 4.91%; O 29.24%

Hazard & Toxicity: LD₅₀ (mus, ipr) 657 mg/kg. Exp. reprod. effects

>>Variant: (*E*)-form

CAS Registry Number: 501-98-4

Molecular Formula: C₉H₈O₃

Molecular Weight: 164.16

Accurate Mass: 164.047345

Percentage Composition: C 65.85%; H 4.91%; O 29.24%

Biological Source: Widespread in plants, e.g. peel of *Prunus serotina*, and from *Trifolium pratense* and *Daviesia latifolia*. Occurs as many glycosides. Found by Bate-Smith in 48% of investigated dicotyledonous and 55% of monocotyledonous spp.

Biological Use/Importance: Shows cytostatic activity

Physical Description: Cryst. + 1H₂O (cold H₂O), anhyd. cryst. (hot H₂O)

Melting Point: Mp 210-213°

Solubility: Sol. Et₂O, hot EtOH; spar. sol. C₆H₆; insol. petrol; BERDY SOL: Sol. MeOH, Et₂O; poorly sol. hexane, C₆H₆

pKa Value: pK_{a1} 4.64; pK_{a2} 9.45 (25°)

UV: [neutral] λ_{max} 225 (); 290 (); 310 () (MeOH) (Berdy) [neutral] λ_{max} 223 (ε 14450); 286 (ε 19000) (EtOH) (Berdy)

Other Data: SOCl₂-activated polycondensation gives the homopolyester with an all-*trans* struct. Polyesters with other hydroxy acids are also known

Aldrich: H2320-1

Fluka: 28200

Sigma: C9008

>>Derivative: *O*-Sulfate

Synonym(s): ***p*-Coumaric acid sulfate**

Molecular Formula: C₉H₈O₆S

Molecular Weight: 244.225

Accurate Mass: 244.00416

Percentage Composition: C 44.26%; H 3.30%; O 39.31%; S 13.13%

Biological Source: Constit. of *Zostera marina*

Use/Importance: Marine antifouling agent

>>Derivative: Me ester

CAS Registry Number: 19367-38-5

Molecular Formula: C₁₀H₁₀O₃

Molecular Weight: 178.187

Accurate Mass: 178.062995

Percentage Composition: C 67.41%; H 5.66%; O 26.94%

Biological Source: Constit. of *Pseudosindora palustris* wood and *Pueraria lobata* callus tissue

Physical Description: Needles (H₂O), tablets (EtOH)

Melting Point: Mp 137°