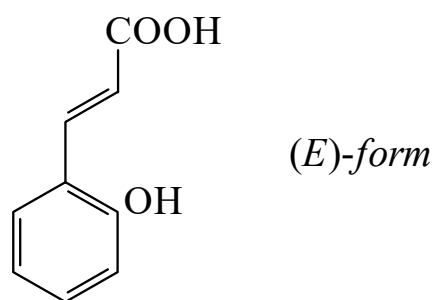




>>Entry Name: 3-(2-Hydroxyphenyl)-2-propenoic acid, 9CI

Synonym(s): *o*-Hydroxycinnamic acid, 8CI. *o*-Cumaric acid. *o*-Coumaric acid



CAS Registry Number: 583-17-5

Related CAS Registry Numbers(s): 6099-03-2 69038-81-9

Molecular Formula: C₉H₈O₃

Molecular Weight: 164.16

Accurate Mass: 164.047345

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

Use/Importance: Used as a 1% soln. in EtOH as a fluorescence acid-base indicator (pH range 7.2-9.0; colour change: non-fluoresc. → green)

pKa Value: p*K*_{a1} 3.7 (30°, 1.0*M* LiCl)

>>Variant: (*E*)-form

CAS Registry Number: 614-60-8

Molecular Formula: C₉H₈O₃

Molecular Weight: 164.16

Accurate Mass: 164.047345

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

Biological Source: Occurs in many plants e.g. *Melilotus officinalis* and *Angraecum fragrans*

Use/Importance: Intermed. in biosynth. of coumarins

Physical Description: Needles (H₂O)

Melting Point: Mp 207-208 dec.°

Solubility: Sol. EtOH, hot H₂O, Et₂O; insol. CS₂, CHCl₃

pKa Value: p*K*_a 4.61

Other Data: Nonvolatile in steam. Dec. on dist.

Hazard & Toxicity: LD₅₀ (mus, ivn) 180 mg/kg

Aldrich: H2280-9

Fluka: 28170

Sigma: C4400

>>Derivative: Ac

Molecular Formula: C₁₁H₁₀O₄

Molecular Weight: 206.198

Accurate Mass: 206.05791

Percentage Composition: C 64.07%; H 4.89%; O 31.04%

Melting Point: Mp 149°

>>Derivative: Me ether

Synonym(s): 3-(2-Methoxyphenyl)-2-propenoic acid. *o*-Methoxycinnamic acid. *O*-Methyl-*o*-coumaric acid

CAS Registry Number: 1011-54-7

Molecular Formula: C₁₀H₁₀O₃

Molecular Weight: 178.187

Accurate Mass: 178.062995

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

Melting Point: Mp 185-186°

pKa Value: p*K*_a 4.78 (25°)

Fluka: 65400