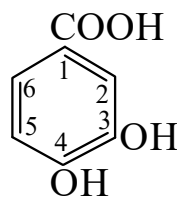




>>Entry Name: 3,4-Dihydroxybenzoic acid

ENTRY UNDER REVIEW

Synonym(s): Protocatechuic acid, 8Cl. Catechol-4-carboxylic acid. Hypogallic acid. Carbohydroquinonic acid



CAS Registry Number: 99-50-3

Related CAS Registry Numbers(s): 58534-64-8

Molecular Formula: C₇H₆O₄

Molecular Weight: 154.122

Accurate Mass: 154.02661

Percentage Composition: C 54.55%; H 3.92%; O 41.52%

Source/Synthesis: Present in red wine

Biological Source: Can be extracted from lignin. Isol. in free state from various higher plants, e.g. *Fagopyrum* and *Alnus* spp.

Biological Use/Importance: Antioxidant, free radical scavenger, dietary chemopreventive agent (inhibits development of neoplasms in animal models), inhibits LDL oxidation, platelet aggregation inhibitor. Shows cytostatic activity

Physical Description: Needles + 1H₂O (H₂O)

Melting Point: Mp 195-196° (anhyd.)

pKa Value: pK_{a1} 4.49; pK_{a2} 8.64; pK_{a3} 1 (25°)

Aldrich: D10980-0

Fluka: 37580

Sigma: P5630

>>Derivative: Me ester

Synonym(s): Methyl 3,4-dihydroxybenzoate

CAS Registry Number: 2150-43-8

Molecular Formula: C₈H₈O₄

Molecular Weight: 168.149

Accurate Mass: 168.04226

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Biological Source: Isol. from stems of *Bauhinia manca*

Biological Use/Importance: Has antimicrobial props.

Physical Description: Needles (H₂O)

Melting Point: Mp 134.5°

pKa Value: pK_{a1} 8.18; pK_{a2} 13.04 (20°)

Other Data: Poss. an artifact

>>Derivative: Et ester

CAS Registry Number: 3943-89-3

Molecular Formula: C₉H₁₀O₄

Molecular Weight: 182.176

Accurate Mass: 182.05791

Percentage Composition: C 59.34%; H 5.53%; O 35.13%

Physical Description: Cryst. (CHCl₃)

Melting Point: Mp 132-134° (128-130°)

Aldrich: E2485-9

Rare Chemicals Library: S43951-7

Sigma: P1653