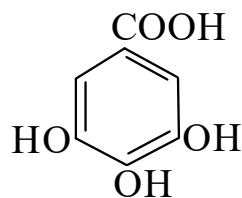




>>Entry Name: 3,4,5-Trihydroxybenzoic acid

ENTRY UNDER REVIEW

Synonym(s): Gallic acid



CAS Registry Number: 149-91-7

Related CAS Registry Numbers(s): 5995-86-8 13405-60-2

Molecular Formula: C₇H₆O₅

Molecular Weight: 170.121

Accurate Mass: 170.021525

Percentage Composition: C 49.42%; H 3.55%; O 47.02%

Biological Source: Isol. by Scheele in 1786 from fermented galls. Occurs in many tannins. Specific flowering inhibitor in leaves of *Kalenchoe bloesfeldiana*. Present in red wine

Use/Importance: Used in tanning, as anal. reagent and photographic developer. Used as 2% soln. in Me₂CO for photometric detn. of Nb (in the presence of aniline), Th, Ti, Ce, Cu

Biological Use/Importance: Antineoplastic agent, astringent. Possesses bacteriostatic activity

Physical Description: Needles (MeOH or CHCl₃); cryst. + 1H₂O (H₂O)

Melting Point: Mp 253 dec.°. Mp 235-240° (225°)

Solubility: Sol. Me₂CO, EtOH; spar. sol. H₂O; insol. C₆H₆, CHCl₃

pKa Value: pK_{a1} 3.13; pK_{a2} 8.84; pK_{a3} 12.4 (20°, 0.1M KNO₃)

Calculated Log P Data: Log P 0.43 (calc)

Hazard & Toxicity: LD₅₀ (rbt, orl) 5000 mg/kg. Exp. reprod. effects

Aldrich: 14791-5

Sigma: G7384

>>Derivative: Me ester

Synonym(s): Methyl 3,4,5-trihydroxybenzoate. Methyl gallate. **Gallicin**‡

CAS Registry Number: 99-24-1

Molecular Formula: C₈H₈O₅

Molecular Weight: 184.148

Accurate Mass: 184.037175

Percentage Composition: C 52.18%; H 4.38%; O 43.44%

Biological Source: Found in *Koelerenteria paniculata*

Melting Point: Mp 157°

Solubility: Sol. MeOH, EtOH, Me₂CO, dioxan, Py, Et₂O; fairly sol. CHCl₃, H₂O; poorly sol. C₆H₆, toluene, hexane, CCl₄

pKa Value: pK_{a1} 7.88 (25°, 0.1M KNO₃)

UV: [neutral] λ_{max} 276 (E1%/1cm 623); 283 () (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, orl) 1700 mg/kg ; LD₅₀ (mus, ivn) 470 mg/kg ; LD₅₀ (mus, ipr) 784 mg/kg

Aldrich: 27419-4

Fluka: 48690

Sigma: M6019

>>Derivative: Et ester

Synonym(s): Ethyl 3,4,5-trihydroxybenzoate. Ethyl gallate. Phyllemblin

CAS Registry Number: 831-61-8

Molecular Formula: C₉H₁₀O₅

Molecular Weight: 198.175

Accurate Mass: 198.052825

Percentage Composition: C 54.55%; H 5.09%; O 40.37%

Biological Source: Occurs, *inter alia*, in *Acacia* spp. and *Phyllanthus emblica*

Biological Use/Importance: Possesses bactericidal props.

Melting Point: Mp 160-162° (anhyd.)

Calculated Log P Data: Log P 1.46 (calc)

Fluka: 48640