



Synonym(s): Propyl 3,4,5-trihydroxybenzoate. Propyl gallate. E 310

CAS Registry Number: 121-79-9

Molecular Formula: C₁₀H₁₂O₅

Molecular Weight: 212.202

Accurate Mass: 212.068475

Percentage Composition: C 56.60%; H 5.70%; O 37.70%

Use/Importance: Used as a 0.1M soln. in aq. Me₂CO for photometric detn. of Nb

Biological Use/Importance: Antioxidant used in food and pharmaceuticals

Physical Description: Cryst.

Melting Point: Mp 150° (147-148°)

Solubility: Sol. Me₂CO, 2-butanol

Hazard & Toxicity: LD₅₀ (rat, orl) 2100 mg/kg. Exp. reprod. and teratogenic effects (v. large doses)

Aldrich: P5330-6

Fluka: 48710

Sigma: P3130

Supelco: R60-0406

>>Derivative: Isopropyl ester

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

CAS Registry Number: 1138-60-9

Molecular Formula: C₁₀H₁₂O₅

Molecular Weight: 212.202

Accurate Mass: 212.068475

Percentage Composition: C 56.60%; H 5.70%; O 37.70%

Physical Description: Cryst. (CHCl₃)

Melting Point: Mp 122-125°

>>Derivative: Butyl ester

CAS Registry Number: 1083-41-6

Molecular Formula: C₁₁H₁₄O₅

Molecular Weight: 226.229

Accurate Mass: 226.084125

Percentage Composition: C 58.40%; H 6.24%; O 35.36%

Physical Description: Needles (toluene)

Melting Point: Mp 142-144°

>>Derivative: 3-Methylbutyl ester

Synonym(s): 3-Methylbutyl 3,4,5-trihydroxybenzoate, 9CI. Isopentyl gallate

CAS Registry Number: 2486-02-4

Molecular Formula: C₁₂H₁₆O₅

Molecular Weight: 240.255

Accurate Mass: 240.099775

Percentage Composition: C 59.99%; H 6.71%; O 33.30%

Physical Description: Needles (H₂O)

Melting Point: Mp 145-146°

>>Derivative: Octyl ester

CAS Registry Number: 1034-01-1

Molecular Formula: C₁₅H₂₂O₅

Molecular Weight: 282.336

Accurate Mass: 282.146725

Percentage Composition: C 63.81%; H 7.85%; O 28.33%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 94-95°