



Molecular Formula: C₁₁H₁₀O₆
Molecular Weight: 238.196
Accurate Mass: 238.04774
Percentage Composition: C 55.47%; H 4.23%; O 40.30%
Physical Description: Needles (C₆H₆)
Melting Point: Mp 162° (157-158°)

>>**Derivative:** 3-Me ether
Synonym(s): 4-Hydroxy-3-methoxybenzoic acid. Vanillic acid

CAS Registry Number: 121-34-6

Molecular Formula: C₈H₈O₄
Molecular Weight: 168.149
Accurate Mass: 168.04226
Percentage Composition: C 57.14%; H 4.80%; O 38.06%
Biological Source: Prod. of alkaline oxid. of chlorite-treated woodpulp. Isol. in free state from various higher plants
Use/Importance: Monomer for polyesters
Physical Description: Needles (H₂O)
Melting Point: Mp 210°
pKa Value: pK_{a1} 4.51; pK_{a2} 9.39 (25°)
Other Data: Sublimes

Aldrich: H3600-1
Fluka: 94770
Sigma: V2250

>>**Derivative:** 3-Me ether, Me ester
Synonym(s): Methyl vanillate

CAS Registry Number: 3943-74-6

Molecular Formula: C₉H₁₀O₄
Molecular Weight: 182.176
Accurate Mass: 182.05791
Percentage Composition: C 59.34%; H 5.53%; O 35.13%
Biological Source: Isol. from stems of *Bauhinia manca*
Physical Description: Needles (EtOH aq.)
Melting Point: Mp 62-63°
Boiling Point: Bp 285-287°
UV: [neutral] λ_{max} 220 (ε 23400); 263 (ε 13500); 293 (ε 7220) (MeOH) (Berdy) [base] λ_{max} 235 (ε 13800); 314 (ε 23450) (MeOH-NAOH) (Berdy)
Other Data: Poss. an artifact

Aldrich: 13812-6

>>**Derivative:** 3-Me ether, Et ester
Synonym(s): Ethyl vanillate

CAS Registry Number: 617-05-0
Molecular Formula: C₁₀H₁₂O₄
Molecular Weight: 196.202
Accurate Mass: 196.07356
Percentage Composition: C 61.22%; H 6.16%; O 32.62%
Physical Description: Needles
Melting Point: Mp 44°
Boiling Point: Bp 291-293°

>>**Derivative:** 3-Me ether, hexyl ester
Synonym(s): Hexyl vanillate

CAS Registry Number: 84375-71-3
Molecular Formula: C₁₄H₂₀O₄
Molecular Weight: 252.31
Accurate Mass: 252.13616
Percentage Composition: C 66.65%; H 7.99%; O 25.36%
Use/Importance: Used in dental cements
Density: d 1.08
Refractive Index: n