



>>Derivative: 3-Me ether, Ac

Synonym(s): 4-(Acetyloxy)-3-methoxybenzoic acid, 9CI

CAS Registry Number: 10543-12-1

Molecular Formula: $C_{10}H_{10}O_5$

Molecular Weight: 210.186

Accurate Mass: 210.052825

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

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 145-146°

Rare Chemicals Library: S37673-6

>>Derivative: 4-Me ether

Synonym(s): 3-Hydroxy-4-methoxybenzoic acid. Isovanillic acid. 3-Hydroxy-*p*-anisic acid

CAS Registry Number: 645-08-9

Molecular Formula: $C_8H_8O_4$

Molecular Weight: 168.149

Accurate Mass: 168.04226

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

Biological Source: Isol. from leaves of *Hydrangea macrophylla*

Physical Description: Prisms, needles or plates (H_2O)

Melting Point: Mp 255-257 subl.°

pKa Value: pK_{a1} 4.47; pK_{a2} 10.1 (25°)

Aldrich: 22010-8

Sigma: I5878

>>Derivative: 4-Me ether, Me ester

Synonym(s): Methyl isovanillate

CAS Registry Number: 6702-50-7

Molecular Formula: $C_9H_{10}O_4$

Molecular Weight: 182.176

Accurate Mass: 182.05791

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

Physical Description: Cryst. (petrol/ Et_2O)

Melting Point: Mp 65.5-66°

Aldrich: 47070-8

>>Derivative: Di-Me ether

see 3,4-Dimethoxybenzoic acid, [DZS04-N](#)

>>Derivative: 3-Et ether

Synonym(s): 3-Ethoxy-4-hydroxybenzoic acid, 9CI

CAS Registry Number: 5438-38-0

Molecular Formula: $C_9H_{10}O_4$

Molecular Weight: 182.176

Accurate Mass: 182.05791

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

Physical Description: Cryst. (H_2O)

Melting Point: Mp 163-164°

>>Derivative: 3-Et ether, 4-Me ether

Synonym(s): 3-Ethoxy-4-methoxybenzoic acid, 9CI

CAS Registry Number: 2651-55-0

Molecular Formula: $C_{10}H_{12}O_4$

Molecular Weight: 196.202

Accurate Mass: 196.07356

Percentage Composition: C 61.22%; H 6.16%; O 32.62%

Physical Description: Cryst. (EtOAc/ C_6H_6)

Melting Point: Mp 164-164.5°