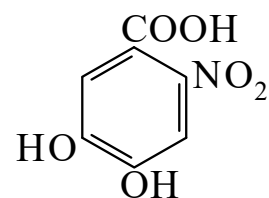




>>Entry Name: 4,5-Dihydroxy-2-nitrobenzoic acid, 9CI

Synonym(s): 6-Nitropyrocatechuic acid, 8CI



Related CAS Registry Numbers(s): 26791-93-5

Molecular Formula: C₇H₅NO₆

Molecular Weight: 199.12

Accurate Mass: 199.011689

Percentage Composition: C 42.22%; H 2.53%; N 7.03%; O 48.21%

>>Derivative: 4-Me ether

Synonym(s): 5-Hydroxy-4-methoxy-2-nitrobenzoic acid. 6-Nitroisovanillic acid

CAS Registry Number: 31839-20-0

Molecular Formula: C₈H₇NO₆

Molecular Weight: 213.146

Accurate Mass: 213.027339

Percentage Composition: C 45.08%; H 3.31%; N 6.57%; O 45.04%

Physical Description: Yellow prisms (H₂O)

Melting Point: Mp 181 dec.°

>>Derivative: 4-Me ether, Me ester

Molecular Formula: C₉H₉NO₆

Molecular Weight: 227.173

Accurate Mass: 227.042989

Percentage Composition: C 47.58%; H 3.99%; N 6.17%; O 42.26%

Melting Point: Mp 143°

>>Derivative: 5-Me ether

Synonym(s): 4-Hydroxy-5-methoxy-2-nitrobenzoic acid. 6-Nitrovanillic acid

Molecular Formula: C₈H₇NO₆

Molecular Weight: 213.146

Accurate Mass: 213.027339

Percentage Composition: C 45.08%; H 3.31%; N 6.57%; O 45.04%

Biological Source: Constit. of a *Cortinarius* sp.

Physical Description: Pale-yellow needles (EtOAc/petrol)

Melting Point: Mp 181-182°

>>Derivative: Di-Me ether

Synonym(s): 4,5-Dimethoxy-2-nitrobenzoic acid

CAS Registry Number: 4998-07-6

Molecular Formula: C₉H₉NO₆

Molecular Weight: 227.173

Accurate Mass: 227.042989

Percentage Composition: C 47.58%; H 3.99%; N 6.17%; O 42.26%

Physical Description: Yellow needles + ½ H₂O

Melting Point: Mp 189-191°

pKa Value: pK_a 2.44 (25°)

Aldrich: 32923-1

>>Derivative: Di-Me ether, Me ester

Molecular Formula: C₁₀H₁₁NO₆

Molecular Weight: 241.2

Accurate Mass: 241.058639

Percentage Composition: C 49.80%; H 4.60%; N 5.81%; O 39.80%

Melting Point: Mp 141-144°