



>>Entry Name: 4-Amino-1,2-benzenediol, 9CI

Synonym(s): 4-Aminopyrocatechol. 3,4-Dihydroxyaniline

CAS Registry Number: 13047-04-6

Molecular Formula: $C_6H_7NO_2$

Molecular Weight: 125.127

Accurate Mass: 125.047679

Percentage Composition: C 57.59%; H 5.64%; N 11.19%; O 25.57%

Biological Use/Importance: Sympathomimetic in animals

pKa Value: pK_{a1} 8.12; pK_{a2} 10.65; pK_{a3} 12.11 (20°)

Other Data: Apparently unstable

Hazard & Toxicity: Nephrotoxic

>>Derivative: Hydrochloride

CAS Registry Number: 4956-56-3

Melting Point: Mp 224-227°

>>Derivative: 2-Benzenesulfonyl

CAS Registry Number: 36383-38-7

Physical Description: Flakes (C_6H_6)

Melting Point: Mp 140-141°

>>Derivative: 1-Ac, 2-benzenesulfonyl

CAS Registry Number: 36383-41-2

Physical Description: Prisms (MeOH)

Melting Point: Mp 135-136°

>>Derivative: 1-Me ether

Synonym(s): 5-Amino-2-methoxyphenol, 9CI. 5-Aminoguaiacol. 4-Aminoguaiacol

CAS Registry Number: 1687-53-2

Molecular Formula: $C_7H_9NO_2$

Molecular Weight: 139.154

Accurate Mass: 139.063329

Percentage Composition: C 60.42%; H 6.52%; N 10.07%; O 23.00%

Physical Description: Grey cryst. (C_6H_6)

Melting Point: Mp 131-133° (125-127°)

Aldrich: 26211-0