



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

>>Derivative: 1-Me ether; hydrochloride

CAS Registry Number: 35589-31-2
Physical Description: Green prisms (HCl)
Melting Point: Mp 160-180 dec.°

>>Derivative: 1-Me ether, 2-Ac

CAS Registry Number: 53606-43-2
Molecular Formula: $C_9H_{11}NO_3$
Molecular Weight: 181.191
Accurate Mass: 181.073894
Percentage Composition: C 59.66%; H 6.12%; N 7.73%; O 26.49%
Physical Description: Needles (EtOAc/petrol)
Melting Point: Mp 81°
Other Data: Darkens in air