



>>Entry Name: 4-Amino-1,3-benzenediol, 9Cl
Synonym(s): 4-Aminoresorcinol, 8Cl. 2,4-Dihydroxyaniline

CAS Registry Number: 13066-95-0
Related CAS Registry Numbers(s): 37966-57-7

Molecular Formula: C₆H₇NO₂
Molecular Weight: 125.127
Accurate Mass: 125.047679
Percentage Composition: C 57.59%; H 5.64%; N 11.19%; O 25.57%
Use/Importance: Used in hair dyes
pKa Value: pK_{a1} 7.91; pK_{a2} 9.16; pK_{a3} 11.24 (20°)
Other Data: Unstable

>>Derivative: Hydrochloride

CAS Registry Number: 34781-86-7
Physical Description: Cryst. + 2H₂O
Aldrich: 16317-1

>>Derivative: *N*-Ac

CAS Registry Number: 71516-07-9
Molecular Formula: C₈H₉NO₃
Molecular Weight: 167.164
Accurate Mass: 167.058244
Percentage Composition: C 57.48%; H 5.43%; N 8.38%; O 28.71%
Melting Point: Mp 164-165°

>>Derivative: *O,O,N*-Tri-Ac

CAS Registry Number: 71516-10-4
Molecular Formula: C₁₂H₁₃NO₅
Molecular Weight: 251.238
Accurate Mass: 251.079374
Percentage Composition: C 57.37%; H 5.22%; N 5.58%; O 31.84%
Melting Point: Mp 114°

>>Derivative: 1-Me ether
Synonym(s): 2-Amino-5-methoxyphenol

CAS Registry Number: 40925-70-0
Molecular Formula: C₇H₉NO₂
Molecular Weight: 139.154
Accurate Mass: 139.063329
Percentage Composition: C 60.42%; H 6.52%; N 10.07%; O 23.00%
Physical Description: Prisms (EtOAc), cryst. (Et₂O)
Melting Point: Mp 128-130°
Other Data: Turns red in light. Unstable in acids, stable in desiccator under Ar

>>Derivative: 1-Me ether; hydrochloride

CAS Registry Number: 39547-15-4
Physical Description: Needles (HCl aq.)
Melting Point: Mp 205-206° (214°)

>>Derivative: 1-Me ether, *N*-Ac

CAS Registry Number: 58469-06-0
Molecular Formula: C₉H₁₁NO₃
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 (H₂O)
Melting Point: Mp 164-165°
Rare Chemicals Library: S67181-9