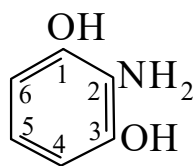




>>Entry Name: 2-Amino-1,3-benzenediol, 9Cl

Synonym(s): 2-Aminoresorcinol, 8Cl. 2,6-Dihydroxyaniline



CAS Registry Number: 3163-15-3

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%

General Statement: Free base unstable

Use/Importance: Used in hair dyes

Physical Description: Brown solid

pKa Value: pK_{a1} 8.09; pK_{a2} 9.35; pK_{a3} 11.58 (20°) pK_{a1} 5.1; pK_{a2} 9.3; pK_{a3} 11.6 (23°)

Hazard & Toxicity: Nephrotoxic

>>Derivative: Hydrochloride

CAS Registry Number: 634-60-6

Melting Point: Mp 240 dec.°

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

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%

Physical Description: Cryst. (MeOH/Et₂O)

Melting Point: Mp 164-165°

>>Derivative: Mono-Me ether

Synonym(s): 2-Amino-3-methoxyphenol, 9Cl. 2-Hydroxy-6-methoxyaniline

CAS Registry Number: 40925-69-7

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%

Melting Point: Mp 123°

>>Derivative: Di-Me ether

Synonym(s): 2,6-Dimethoxyaniline

CAS Registry Number: 2734-70-5

Molecular Formula: C₈H₁₁NO₂

Molecular Weight: 153.18

Accurate Mass: 153.078979

Percentage Composition: C 62.73%; H 7.24%; N 9.14%; O 20.89%

Physical Description: Leaflets (petrol)

Melting Point: Mp 75°

Boiling Point: Bp₂₃ 146°

>>Derivative: Di-Me ether, N-Ac

Molecular Formula: C₁₀H₁₃NO₃

Molecular Weight: 195.218

Accurate Mass: 195.089544

Percentage Composition: C 61.53%; H 6.71%; N 7.17%; O 24.59%

Physical Description: Plates (H₂O or AcOH)

Melting Point: Mp 81°