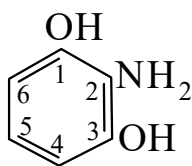




>>Entry Name: 2-Amino-1,3-benzenediol, 9Cl

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



CAS Registry Number: 3163-15-3

Molecular Formula: C<sub>6</sub>H<sub>7</sub>NO<sub>2</sub>

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<sub>a1</sub> 8.09; pK<sub>a2</sub> 9.35; pK<sub>a3</sub> 11.58 (20°) pK<sub>a1</sub> 5.1; pK<sub>a2</sub> 9.3; pK<sub>a3</sub> 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: C<sub>12</sub>H<sub>13</sub>NO<sub>5</sub>

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/Et<sub>2</sub>O)

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: C<sub>7</sub>H<sub>9</sub>NO<sub>2</sub>

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: C<sub>8</sub>H<sub>11</sub>NO<sub>2</sub>

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: Bp<sub>23</sub> 146°

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

Molecular Formula: C<sub>10</sub>H<sub>13</sub>NO<sub>3</sub>

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 (H<sub>2</sub>O or AcOH)

Melting Point: Mp 81°