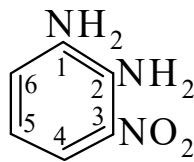




>>Entry Name: 1,2-Diamino-3-nitrobenzene

Synonym(s): 3-Nitro-1,2-benzenediamine, 9Cl. 3-Nitro-*o*-phenylenediamine, 8Cl



CAS Registry Number: 3694-52-8

Molecular Formula: C₆H₇N₃O₂

Molecular Weight: 153.14

Accurate Mass: 153.053827

Percentage Composition: C 47.06%; H 4.61%; N 27.44%; O 20.90%

Physical Description: Dark red needles (EtOH aq.)

Melting Point: Mp 158-159°

Aldrich: N2130-8

Fluka: 73625

>>Derivative: 1-*N*-Ac

CAS Registry Number: 76320-87-1

Molecular Formula: C₈H₉N₃O₃

Molecular Weight: 195.177

Accurate Mass: 195.064392

Percentage Composition: C 49.23%; H 4.65%; N 21.53%; O 24.59%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 158-160° (165-167°)

>>Derivative: 1-*N*-Benzoyl

Molecular Formula: C₁₃H₁₁N₃O₃

Molecular Weight: 257.248

Accurate Mass: 257.080042

Percentage Composition: C 60.70%; H 4.31%; N 16.33%; O 18.66%

Physical Description: Dark yellow needles (EtOH)

Melting Point: Mp 206°

>>Derivative: 2-*N*-Me

CAS Registry Number: 13183-00-1

Molecular Formula: C₇H₉N₃O₂

Molecular Weight: 167.167

Accurate Mass: 167.069477

Percentage Composition: C 50.30%; H 5.43%; N 25.14%; O 19.14%

Melting Point: Mp 75-76°

>>Derivative: 2-*N*-Di-Me

Molecular Formula: C₈H₁₁N₃O₂

Molecular Weight: 181.194

Accurate Mass: 181.085127

Percentage Composition: C 53.03%; H 6.12%; N 23.19%; O 17.66%

Physical Description: Dark red mass

>>Derivative: 2-*N*-Di-Me, 1-*N*-benzoyl

Molecular Formula: C₁₅H₁₅N₃O₃

Molecular Weight: 285.302

Accurate Mass: 285.111342

Percentage Composition: C 63.15%; H 5.30%; N 14.73%; O 16.82%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 114°

References: