



>>Entry Name: 1,4-Diamino-2-nitrobenzene

Synonym(s): 2-Nitro-1,4-benzenediamine, 9CI. 2-Nitro-*p*-phenylenediamine, 8CI

CAS Registry Number: 5307-14-2

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%

Use/Importance: Used in hair dyes. Comonomer for polyamides

Physical Description: Black needles with strong green reflex (H₂O)

Melting Point: Mp 137°

Hazard & Toxicity: LD₅₀ (rat, orl) 3080 mg/kg. Exp. reprod. and teratogenic effects. Mutagenic props

Aldrich: N2120-0

Fluka: 73620

Sigma: N4757

>>Derivative: 1-*N*-Ac

Synonym(s): 4-Amino-2-nitroacetanilide

CAS Registry Number: 7418-43-1

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: Red needles (H₂O), dark-red and orange cryst. (EtOH)

Melting Point: Mp 162.5°. Mp 165-166°

Rare Chemicals Library: S73136-6

>>Derivative: 4-*N*-Ac

Synonym(s): 4-Amino-3-nitroacetanilide

CAS Registry Number: 6086-29-9

Physical Description: Red needles or leaflets (H₂O)

Melting Point: Mp 189°

Rare Chemicals Library: S3415-1

>>Derivative: 1,4-Di-Ac

CAS Registry Number: 5345-53-9

Molecular Formula: C₁₀H₁₁N₃O₄

Molecular Weight: 237.215

Accurate Mass: 237.074957

Percentage Composition: C 50.63%; H 4.67%; N 17.71%; O 26.98%

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 186°

Rare Chemicals Library: S80406-1

>>Derivative: 4-*N*-Benzoyl

CAS Registry Number: 27908-96-9

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: Orange needles

Melting Point: Mp 236°