



>>Entry Name: 4-Methyl-3-nitroaniline

Synonym(s): 4-Methyl-3-nitrobenzenamine, 9Cl. 3-Nitro-*p*-toluidine, 8Cl. 4-Amino-2-nitrotoluene

CAS Registry Number: 119-32-4

Molecular Formula: C₇H₈N₂O₂

Molecular Weight: 152.152

Accurate Mass: 152.058578

Percentage Composition: C 55.26%; H 5.30%; N 18.41%; O 21.03%

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 78°

pKa Value: pK_a 3.02 (25°)

Hazard & Toxicity: Fl. p. >71°

Aldrich: M5980-7

Sigma: M4013

>>Derivative: Hydrochloride

Physical Description: Cryst.

Melting Point: Mp 230-240°

>>Derivative: *N*-Formyl

Molecular Formula: C₈H₈N₂O₃

Molecular Weight: 180.163

Accurate Mass: 180.053493

Percentage Composition: C 53.33%; H 4.48%; N 15.55%; O 26.64%

Physical Description: Cryst.

Melting Point: Mp 133-134°

>>Derivative: *N*-Ac

Molecular Formula: C₉H₁₀N₂O₃

Molecular Weight: 194.19

Accurate Mass: 194.069143

Percentage Composition: C 55.67%; H 5.19%; N 14.43%; O 24.72%

Physical Description: Yellow cryst. (H₂O)

Melting Point: Mp 144-145°

>>Derivative: *N*-Me

Molecular Formula: C₈H₁₀N₂O₂

Molecular Weight: 166.179

Accurate Mass: 166.074228

Percentage Composition: C 57.82%; H 6.07%; N 16.86%; O 19.26%

Physical Description: Red cryst. (EtOH)

Melting Point: Mp 56°

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

Molecular Formula: C₉H₁₂N₂O₂

Molecular Weight: 180.206

Accurate Mass: 180.089878

Percentage Composition: C 59.99%; H 6.71%; N 15.55%; O 17.76%

Physical Description: Orange-red cryst. (EtOH)

Melting Point: Mp 38°

Other Data: Steam-volatile

>>Derivative: *N,N*-Di-Et