



>>Entry Name: 5-Methyl-2-nitroaniline

Synonym(s): 2-Nitro-5-methylbenzenamine, 9Cl. 6-Nitro-*m*-toluidine, 8Cl

CAS Registry Number: 578-46-1

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 cryst. (EtOH aq.)

Melting Point: Mp 110°

pKa Value: pK_a -0.09 (25°)

Aldrich: 26166-1

>>Derivative: N-Ac

Synonym(s): 5-Methyl-2-nitroacetanilide. 6-Nitroacet-*m*-toluidide

CAS Registry Number: 7418-36-2

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 or petrol)

Melting Point: Mp 87°

>>Derivative: N-Benzoyl

Molecular Formula: C₁₄H₁₂N₂O₃

Molecular Weight: 256.26

Accurate Mass: 256.084793

Percentage Composition: C 65.62%; H 4.72%; N 10.93%; O 18.73%

Physical Description: Cryst.

Melting Point: Mp 83°

>>Derivative: N-Me

CAS Registry Number: 65081-42-7

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: Brownish-yellow prisms (MeOH aq.)

Melting Point: Mp 83° (69°)

>>Derivative: N,N-Di-Me

Physical Description: Yellow parallelipeds (MeOH)

Melting Point: Mp 41°

Boiling Point: Bp₃ 128°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 741C, (*nmr*)
Kenner, J. *et al.*, *J.C.S.*, 1920, **117**, 858, (*synth*)
Mangini, A. *et al.*, *Gazz. Chim. Ital.*, 1938, **68**, 543; *CA*, **33**, 3769, (*derivs*)
Hancock, C.K. *et al.*, *J.O.C.*, 1968, **33**, 1947, (*synth*)
Collins, M.J. *et al.*, *Aust. J. Chem.*, 1992, **45**, 1119, (*pmr*)
Skibo, E.B. *et al.*, *J. Med. Chem.*, 1994, **37**, 78, (*N-Me, ir, pmr*)