



>>Entry Name: 4-Chloro-2-nitroaniline, 8Cl
Synonym(s): 4-Chloro-2-nitrobenzenamine, 9Cl

CAS Registry Number: 89-63-4

Molecular Formula: C₆H₅ClN₂O₂
Molecular Weight: 172.57
Accurate Mass: 172.003955
Percentage Composition: C 41.76%; H 2.92%; Cl 20.54%; N 16.23%; O 18.54%
Physical Description: Orange-yellow needles (H₂O)
Melting Point: Mp 116-117°
pKa Value: pK_{a1} -0.99 (25°, H₂SO₄ aq.)

Hazard & Toxicity: Forms explosive prods. with HNO₃. Skin absorption may cause dermatitis, methaemoglobinaemia leading to cyanosis, liver and kidney damage.
Symptoms of exposure may be delayed

Aldrich: 10166-4

Fluka: 25380

Supelco: R30-1385

>>Derivative: N-Ac

CAS Registry Number: 881-51-6
Molecular Formula: C₈H₇ClN₂O₃
Molecular Weight: 214.608
Accurate Mass: 214.01452
Percentage Composition: C 44.77%; H 3.29%; Cl 16.52%; N 13.05%; O 22.37%
Physical Description: Yellow needles (EtOH)
Melting Point: Mp 104°

>>Derivative: N-Me

CAS Registry Number: 15950-17-1
Molecular Formula: C₇H₇ClN₂O₂
Molecular Weight: 186.597
Accurate Mass: 186.019605
Percentage Composition: C 45.06%; H 3.78%; Cl 19.00%; N 15.01%; O 17.15%
Physical Description: Orange cryst. (EtOH)
Melting Point: Mp 110°

>>Derivative: N,N-Di-Me

CAS Registry Number: 17815-99-5
Molecular Formula: C₈H₉ClN₂O₂
Molecular Weight: 200.624
Accurate Mass: 200.035255
Percentage Composition: C 47.89%; H 4.52%; Cl 17.67%; N 13.96%; O 15.95%
Physical Description: Orange-yellow needles (EtOH)
Melting Point: Mp 57°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 744C, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1366C, (*ir*)
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McMaster, L. *et al.*, *Ind. Eng. Chem.*, 1930, **22**, 547, (*synth*)
Appleton, J.M. *et al.*, *Aust. J. Chem.*, 1970, **23**, 1667, (*pmr*)
Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th edn., Van Nostrand Reinhold, 1979, 495
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, 1992, 312