



>>Entry Name: 4-Chloro-2-methylaniline

Synonym(s): 4-Chloro-2-methylbenzenamine, 9CI. 4-Chloro-*o*-toluidine. 2-Amino-5-chlorotoluene

CAS Registry Number: 95-69-2

Related CAS Registry Numbers(s): 27165-08-8

Molecular Formula: C₇H₈ClN

Molecular Weight: 141.6

Accurate Mass: 141.034526

Percentage Composition: C 59.38%; H 5.69%; Cl 25.04%; N 9.89%

Physical Description: Leaflets (EtOH)

Melting Point: Mp 29-30°

Boiling Point: Bp₇₃₀ 236-238°

pKa Value: pK_{a1} 3.85 (25°)

Hazard & Toxicity: CuCl₂-catalysed thermal dec. occurs above 239°. The reaction product of diazotised 4-Chloro-2-methylaniline with Na₂S, NaSH and Na polysulfide solns. is explosive. Probable human carcinogen

Aldrich: C5110-5

Fluka: 25080

Sigma: F0505

>>Derivative: N-Ac

CAS Registry Number: 5202-86-8

Molecular Formula: C₉H₁₀ClNO

Molecular Weight: 183.637

Accurate Mass: 183.045091

Percentage Composition: C 58.87%; H 5.49%; Cl 19.31%; N 7.63%; O 8.71%

Physical Description: Pearly leaflets

Melting Point: Mp 140°

Rare Chemicals Library: S74484-0

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 504A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1219B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1139C, (*ir*)

Nawiasky, P. *et al.*, *Chem. Eng. News*, 1945, **23**, 1247, (*haz*)

Gassman, P.G. *et al.*, *J.A.C.S.*, 1974, **96**, 5487, (*synth*)

Sharma, S.N. *et al.*, *Indian J. Phys.*, 1976, **50**, 25, (*ir*)

IARC Monog., 1978, **16**, 277; 1983, **30**, 65; *Suppl.* 7, 60, (*rev, tox*)

Shashidhar, M.A., *Indian J. Phys.*, 1978, **52**, 125, (*uv*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, CLK220

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 2614