



>>Entry Name: 3-Chloro-2-methylaniline

Synonym(s): 3-Chloro-2-methylbenzenamine, 9Cl. 3-Chloro-*o*-toluidine. 2-Amino-6-chlorotoluene

CAS Registry Number: 87-60-5

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%

Boiling Point: Bp 245°

Other Data: Steam-volatile. Rapidly turns brown in air

Hazard & Toxicity: LD₅₀ (rat, orl) 574 mg/kg

Aldrich: 10162-1

Fluka: 25060

Rare Chemicals Library: S43075-7

Sigma: F9004

>>Derivative: Hydrochloride

CAS Registry Number: 6259-40-1

Melting Point: Mp 250-252 dec.°

>>Derivative: *N*-Ac

Synonym(s): 3-Chloro-2-methylacetanilide. 2-Acetamido-6-chlorotoluene

CAS Registry Number: 7463-35-6

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%

Melting Point: Mp 136°. Mp 157-159°

Aldrich: 46294-2

Rare Chemicals Library: S51565-5

>>Derivative: *N*-Benzoyl

CAS Registry Number: 40447-04-9

Molecular Formula: C₁₄H₁₂ClNO

Molecular Weight: 245.708

Accurate Mass: 245.060741

Percentage Composition: C 68.44%; H 4.92%; Cl 14.43%; N 5.70%; O 6.51%

Melting Point: Mp 165°. Mp 173°

Rare Chemicals Library: S89062-6

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1214A, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1132C, (*ir*)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 1019D, (*nmr*)

Noelting, E., *Ber.*, 1904, **37**, 1015, (*synth, bibl*)

Epstein, E. *et al.*, *J. Pharm. Sci.*, 1960, **49**, 80, (*derivs*)

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

Schimelpfenig, C.W., *J.C.S. Perkin I*, 1977, 1129, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, CLK200