



>>Entry Name: 3-Chloro-2-methylbenzoic acid, 9Cl

Synonym(s): 3-Chloro-*o*-toluic acid

CAS Registry Number: 7499-08-3

Molecular Formula: C₈H₇ClO₂

Molecular Weight: 170.595

Accurate Mass: 170.013457

Percentage Composition: C 56.33%; H 4.14%; Cl 20.78%; O 18.76%

Physical Description: Needles

Melting Point: Mp 163° (154°, 159°)

pKa Value: pK_a 3.43 (20°, 1% EtOH)

Hazard & Toxicity: LD₅₀ (mus, ipr) 422 mg/kg

>>Derivative: Nitrile

Synonym(s): 3-Chloro-2-methylbenzonitrile, 9Cl. 1-Chloro-3-cyano-2-methylbenzene. 2-Chloro-6-cyanotoluene

CAS Registry Number: 54454-12-5

Molecular Formula: C₈H₆ClN

Molecular Weight: 151.595

Accurate Mass: 151.018876

Percentage Composition: C 63.38%; H 3.99%; Cl 23.39%; N 9.24%

Melting Point: Mp 19°

Boiling Point: Bp₂₈ 107°

References:

Nölting, E., *Ber.*, 1904, **37**, 1015-1028, (*synth*)

Peltier, D. *et al.*, *Bull. Soc. Chim. Fr.*, 1960, 1141-1147, (*ir*)

Mitchell, R.H. *et al.*, *J.O.C.*, 1984, **49**, 2534-2540, (*nitrile, synth, pmr, ir*)

Epsztajn, J. *et al.*, *Monatsh. Chem.*, 1992, **123**, 1125-1134, (*synth, ir, pmr*)

Bennetau, B. *et al.*, *J.C.S. Perkin 1*, 1995, 1265-1271, (*synth, pmr, cmr*)