



>>Entry Name: 2-Chloro-6-methylbenzoic acid, 9Cl

Synonym(s): 6-Chloro-*o*-toluic acid

CAS Registry Number: 21327-86-6

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 (H₂O)

Melting Point: Mp 110° (102°, 105°)

pKa Value: pK_a 2.75 (20°, 1% EtOH) pK_a 2.43 (25°, H₂O)

>>Derivative: Chloride

Molecular Formula: C₈H₆Cl₂O

Molecular Weight: 189.04

Accurate Mass: 187.979569

Percentage Composition: C 50.83%; H 3.20%; Cl 37.51%; O 8.46%

Boiling Point: Bp₁₆ 114-116°

>>Derivative: Amide

CAS Registry Number: 101080-58-4

Molecular Formula: C₈H₈ClNO

Molecular Weight: 169.61

Accurate Mass: 169.029441

Percentage Composition: C 56.65%; H 4.75%; Cl 20.90%; N 8.26%; O 9.43%

Physical Description: Scales

Melting Point: Mp 167°

>>Derivative: Nitrile

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

CAS Registry Number: 6575-09-3

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%

Physical Description: Prisms (petrol)

Melting Point: Mp 83-85°

Aldrich: 12508-3

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 454B, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1527A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1416A, (*ir*)
Kenner, J. *et al.*, *J.C.S.*, 1921, **119**, 1452-1461, (*synth*)
Gleu, K. *et al.*, *J. Prakt. Chem.*, 1939, **153**, 200-204, (*synth*)
Häring, M., *Helv. Chim. Acta*, 1960, **43**, 104-113, (*synth*)
Honkanen, E., *CA*, 1961, **55**, 15400d, (*synth*)
Bennetau, B. *et al.*, *J.C.S. Perkin 1*, 1995, 1265-1271, (*synth, pmr*)