



>>Entry Name: 4-Chloro-2-methylbenzoic acid, 9Cl

Synonym(s): 4-Chloro-*o*-toluic acid

CAS Registry Number: 7499-07-2

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 172°

pKa Value: pK_{a1} 3.75 (20°, 1% EtOH)

Other Data: Steam-volatile

>>Derivative: Et ester

CAS Registry Number: 15393-58-5

Molecular Formula: C₁₀H₁₁ClO₂

Molecular Weight: 198.648

Accurate Mass: 198.044757

Percentage Composition: C 60.46%; H 5.58%; Cl 17.85%; O 16.11%

Boiling Point: Bp 258°. Bp₁₄ 132°

Density: d₄²⁵ 1.163

>>Derivative: Amide

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%

Melting Point: Mp 183°

>>Derivative: Nitrile

Synonym(s): 4-Chloro-2-methylbenzonitrile. 4-Chloro-1-cyano-2-methylbenzene. 5-Chloro-2-cyanotoluene

CAS Registry Number: 50712-68-0

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 67°

Other Data: Steam-volatile

References:

- v. Auwers, K. *et al.*, *Z. Phys. Chem., Abt. A*, 1929, **143**, 1-20, (*synth, bibl*)
Peltier, D. *et al.*, *Bull. Soc. Chim. Fr.*, 1960, 1141-1147, (*ir*)
Grethe, G. *et al.*, *J.O.C.*, 1968, **33**, 494-503, (*Et ester, synth, pmr*)
Meschino, J.A. *et al.*, *J.O.C.*, 1971, **36**, 3636-3638, (*pmr*)
Collins, M.J. *et al.*, *Aust. J. Chem.*, 1992, **45**, 1119-1134, (*pmr, ms, nitrile*)
Epszajn, J. *et al.*, *Monatsh. Chem.*, 1992, **123**, 1125-1134, (*synth, ir, pmr*)
Baumgarth, M. *et al.*, *J. Med. Chem.*, 1997, **40**, 2017-2034, (*synth*)
Sasson, Y. *et al.*, *Chem. Comm.*, 1998, 73-74, (*synth*)