



>>Entry Name: 4-Chloro-3-methylbenzoic acid, 9Cl

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

CAS Registry Number: 7697-29-2

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 (H₂O, Me₂CO aq. or PhNO₂)

Melting Point: Mp 209-210°

pKa Value: pK_a 4.07 (20°, 1% EtOH)

>>Derivative: Et ester

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 260-265°

>>Derivative: Chloride

CAS Registry Number: 21900-24-3

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: Bp₃ 105°

>>Derivative: Nitrile

Synonym(s): 4-Chloro-3-methylbenzonitrile. 1-Chloro-4-cyano-2-methylbenzene. 2-Chloro-5-cyanotoluene

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: Yellow needles (petrol)

Melting Point: Mp 60-61°

References:

- Mailhe, A., *Bull. Soc. Chim. Fr.*, 1921, **29**, 290-294, (*synth*)
Bergmann, E.D. *et al.*, *J.A.C.S.*, 1959, **81**, 5641-5646, (*synth*)
Peltier, D. *et al.*, *Bull. Soc. Chim. Fr.*, 1960, 1141-1147, (*ir*)
Hoop, G.M. *et al.*, *J.C.S.*, 1962, 4857-4860, (*synth*)
Crandall, E.W. *et al.*, *J.O.C.*, 1967, **32**, 134-136, (*synth*, *uv*)
Krajniak, E.R. *et al.*, *Aust. J. Chem.*, 1973, **26**, 1337-1351, (*uv*, *ir*, *pmr*, *ms*)
Todd, D. *et al.*, *J. Chem. Educ.*, 1988, **65**, 1100-1103, (*synth*)