



>>Entry Name: 2-Chloro-5-methylbenzoic acid, 9Cl

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

CAS Registry Number: 6342-60-5

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: Cryst. (H₂O)

Melting Point: Mp 150° (147-148°)

pKa Value: pK_a 3.12 (20°, 1% EtOH)

>>Derivative: Me ester

CAS Registry Number: 16220-95-4

Molecular Formula: C₉H₉ClO₂

Molecular Weight: 184.622

Accurate Mass: 184.029107

Percentage Composition: C 58.55%; H 4.91%; Cl 19.20%; O 17.33%

Boiling Point: Bp_{0.8} 79-80°

>>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 186.8-187.6°

>>Derivative: Nitrile

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

CAS Registry Number: 4387-32-0

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 52-54°

References:

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

Koebrich, G. *et al.*, *Annalen*, 1963, **664**, 88-96, (*synth, bibl*)

Collins, M.J. *et al.*, *Aust. J. Chem.*, 1992, **45**, 1119-1134, (*nitrile, synth, pmr*)