



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

Synonym(s): 2-Chloro-*p*-toluic acid

CAS Registry Number: 7697-25-8

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 155-157°

pKa Value: pK_a 3.27 (20°, 1% EtOH)

>>Derivative: Amide

CAS Registry Number: 64597-37-1

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 182°

>>Derivative: Nitrile

Synonym(s): 2-Chloro-4-methylbenzonitrile, 9Cl. 2-Chloro-1-cyano-4-methylbenzene. 3-Chloro-4-cyanotoluene

CAS Registry Number: 21423-84-7

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: Orange cryst.

Melting Point: Mp 51-55° (61-62°)

Other Data: Sublimes. Steam-volatile

References:

de Tar, D.F. *et al.*, *J.A.C.S.*, 1956, **78**, 4302-4305, (*synth*)

Cachia, M. *et al.*, *Bull. Soc. Chim. Fr.*, 1958, 1418-1425, (*synth*)

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

Crandall, E.W. *et al.*, *J.O.C.*, 1967, **32**, 134-136, (*synth*, *uv*)

Otto, J. *et al.*, *Pol. J. Chem. (Rocz. Chem.)*, 1972, **46**, 1551-1558; *CA*, **78**, 57909t, (*synth*)