



>>Entry Name: 5-Amino-2-chlorobenzoic acid, 9Cl, 8Cl

CAS Registry Number: 89-54-3

Molecular Formula: C₇H₆ClNO₂

Molecular Weight: 171.583

Accurate Mass: 171.008706

Percentage Composition: C 49.00%; H 3.52%; Cl 20.66%; N 8.16%; O 18.65%

Physical Description: Needles

Melting Point: Mp 185-188°

Aldrich: 24825-8

Fluka: 7375

>>Derivative: Nitrile

Synonym(s): 4-Chloro-3-cyanoaniline

CAS Registry Number: 35747-58-1

Molecular Formula: C₇H₅ClN₂

Molecular Weight: 152.583

Accurate Mass: 152.014125

Percentage Composition: C 55.10%; H 3.30%; Cl 23.24%; N 18.36%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 133°

>>Derivative: N-Ac

Molecular Formula: C₉H₈ClNO₃

Molecular Weight: 213.62

Accurate Mass: 213.019271

Percentage Composition: C 50.60%; H 3.77%; Cl 16.60%; N 6.56%; O 22.47%

Melting Point: Mp 215°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 218C, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1120A, (*nmr*)

Bergman, E.D. *et al.*, *J.O.C.*, 1961, **26**, 919-923, (*synth*)

Le Guyader, M. *et al.*, *C. R. Hebd. Seances Acad. Sci.*, 1964, **259**, 4719-4721, (*synth*)

Markley, L.D. *et al.*, *J. Med. Chem.*, 1986, **29**, 427-433, (*nitrile, synth*)

Hino, K. *et al.*, *Chem. Pharm. Bull.*, 1988, **36**, 3462-3467, (*synth*)