



>>Entry Name: 2-Chloro-6-nitrobenzoic acid, 9Cl, 8Cl

CAS Registry Number: 5344-49-0

Structure by analogy with 2-Chloro-3-nitrobenzoic acid, [DWX39-F](#)

Molecular Formula: C₇H₄ClNO₄

Molecular Weight: 201.566

Accurate Mass: 200.982886

Percentage Composition: C 41.71%; H 2.00%; Cl 17.59%; N 6.95%; O 31.75%

Physical Description: Cryst.

Melting Point: Mp 160-165°

pKa Value: pK_a 1.34 (25°) pK_a 1.48 (25°, H₂O)

>>Derivative: Me ester

Molecular Formula: C₈H₆ClNO₄

Molecular Weight: 215.592

Accurate Mass: 214.998536

Percentage Composition: C 44.57%; H 2.81%; Cl 16.44%; N 6.50%; O 29.68%

Physical Description: Needles

Melting Point: Mp 94-96°

>>Derivative: Et ester

Molecular Formula: C₉H₈ClNO₄

Molecular Weight: 229.619

Accurate Mass: 229.014186

Percentage Composition: C 47.08%; H 3.51%; Cl 15.44%; N 6.10%; O 27.87%

Physical Description: Cryst.

Melting Point: Mp 49-50°

>>Derivative: Chloride

Molecular Formula: C₇H₃Cl₂NO₃

Molecular Weight: 220.011

Accurate Mass: 218.948998

Percentage Composition: C 38.21%; H 1.37%; Cl 32.23%; N 6.37%; O 21.82%

Physical Description: Cryst. (petrol)

Melting Point: Mp 32-34°

Boiling Point: Bp_{12.5} 160° (lit. gives a pressure range)

>>Derivative: Amide

Molecular Formula: C₇H₅ClN₂O₃

Molecular Weight: 200.581

Accurate Mass: 199.99887

Percentage Composition: C 41.92%; H 2.51%; Cl 17.68%; N 13.97%; O 23.93%

Physical Description: Cryst.

Melting Point: Mp 186-187°

>>Derivative: Nitrile

Synonym(s): 2-Chloro-6-nitrobenzonitrile. 1-Chloro-2-cyano-3-nitrobenzene

CAS Registry Number: 6575-07-1

Molecular Formula: C₇H₃ClN₂O₂

Molecular Weight: 182.566

Accurate Mass: 181.988305

Percentage Composition: C 46.05%; H 1.66%; Cl 19.42%; N 15.34%; O 17.53%

Melting Point: Mp 116-118°

Aldrich: 14225-5

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1528B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 455C, (*ir*)

Goldstein, H. *et al.*, *Helv. Chim. Acta*, 1944, **27**, 612, (*synth*)

McCubbin, J.A. *et al.*, *Can. J. Chem.*, 1970, **48**, 942, (*synth*)