



>>Entry Name: 3-Chloro-2-nitrobenzoic acid, 9Cl, 8Cl

CAS Registry Number: 4771-47-5

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

Molecular Formula: $C_7H_4ClNO_4$

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. (H₂O or EtOH)

Melting Point: Mp 238-239°

pKa Value: pK_a 2.36

Aldrich: 27588-3

Fluka: 25420

>>Derivative: Anilide

Molecular Formula: $C_{13}H_9ClN_2O_3$

Molecular Weight: 276.678

Accurate Mass: 276.03017

Percentage Composition: C 56.43%; H 3.28%; Cl 12.81%; N 10.12%; O 17.35%

Physical Description: Cryst.

Melting Point: Mp 186°

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **2**, 1100B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 207D, (*ir*)

Holleman, A.F. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1901, **20**, 206, (*synth*)

Waters, W.A. *et al.*, *J.C.S.*, 1945, 629, (*synth*)

Unio, S. *et al.*, *Chem. Pharm. Bull.*, 1969, **17**, 596, (*synth*)