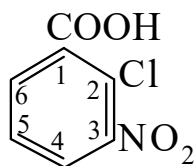




>>Entry Name: 2-Chloro-3-nitrobenzoic acid, 9Cl, 8Cl



CAS Registry Number: 3970-35-2

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. (xylene)

Melting Point: Mp 185°

Aldrich: 14120-8

Fluka: 25408

>>Derivative: Me ester

CAS Registry Number: 53553-14-3

Molecular Formula: $C_8H_6ClNO_4$

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: Cryst. (petrol)

Melting Point: Mp 70°

>>Derivative: Nitrile

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

CAS Registry Number: 34662-24-3

Molecular Formula: $C_7H_3ClN_2O_2$

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%

Physical Description: Pale-yellow cryst.

Melting Point: Mp 97-101°

References:

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

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Kenner, J. *et al.*, *J.C.S.*, 1921, **119**, 598, (*synth*)

Sbarbati, N.E. *et al.*, *J.O.C.*, 1965, **30**, 3365, (*synth*)