



>>Entry Name: 2-Chloro-5-nitrobenzoic acid, 9Cl, 8Cl

CAS Registry Number: 2516-96-3

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. (H_2O)

Melting Point: Mp 165-166°

pKa Value: pK_a 2.19

Aldrich: 12511-3

Fluka: 25415

>>Derivative: Me ester

CAS Registry Number: 6307-82-0

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. (MeOH)

Melting Point: Mp 73°

Hazard & Toxicity: Skin and eye irritant. LD₅₀ (rat, orl) 5360 mg/kg

>>Derivative: Chloride

CAS Registry Number: 25784-91-2

Molecular Formula: $C_7H_3Cl_2NO_3$

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 60°

Boiling Point: Bp₁₁ 157-158°

>>Derivative: Amide

CAS Registry Number: 16588-15-1

Molecular Formula: $C_7H_5ClN_2O_3$

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. (H_2O)

Melting Point: Mp 178°

Rare Chemicals Library: S61395-9

>>Derivative: Nitrile

Synonym(s): 1-Chloro-2-cyano-4-nitrobenzene

CAS Registry Number: 16588-02-6

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: Cryst.

Melting Point: Mp 105-106°

Aldrich: 13571-2

References: