>>**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. LD_{50} (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: Bp_{11} 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: