>>**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: $C_7H_4ClNO_4$
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.
Melting Point: Mp 160-165°
pKa Value: pK_a 1.34 (25°) pK_a 1.48 (25°, H_2O)

>>**Derivative:** Me ester

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: Needles
Melting Point: Mp 94-96°

>>**Derivative:** Et ester

Molecular Formula: $C_9H_8ClNO_4$
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: $C_7H_3Cl_2NO_3$
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 32-34°
Boiling Point: $Bp_{12.5}$ 160° (lit. gives a pressure range)

>>**Derivative:** Amide

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.
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: $C_7H_3ClN_2O_2$
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%
Melting Point: Mp 116-118°
Aldrich: 14225-5

References:

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