



>>Entry Name: 4-Chloro-2-nitrobenzoic acid, 9Cl, 8Cl

CAS Registry Number: 6280-88-2

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

Molecular Formula: C₇H₄ClNO₄

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 C₆H₆)

Melting Point: Mp 142°

pKa Value: pK_a 2

Aldrich: C5980-7

Fluka: 25440

Sigma: C4878

>>Derivative: Me ester

CAS Registry Number: 42087-80-9

Molecular Formula: C₈H₆ClNO₄

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.

Melting Point: Mp 41-43°

Aldrich: 21735-2

>>Derivative: Chloride

Molecular Formula: C₇H₃Cl₂NO₃

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.

Melting Point: Mp 31-34°

>>Derivative: Amide

CAS Registry Number: 41994-91-6

Molecular Formula: C₇H₅ClN₂O₃

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. (EtOH)

Melting Point: Mp 172°

>>Derivative: Nitrile

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

CAS Registry Number: 34662-32-3

Molecular Formula: C₇H₃ClN₂O₂

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 98°

Rare Chemicals Library: S74497-2

References:

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