



>>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: C<sub>7</sub>H<sub>4</sub>ClNO<sub>4</sub>

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<sub>2</sub>O or C<sub>6</sub>H<sub>6</sub>)

Melting Point: Mp 142°

pKa Value: pK<sub>a</sub> 2

Aldrich: C5980-7

Fluka: 25440

Sigma: C4878

>>Derivative: Me ester

CAS Registry Number: 42087-80-9

Molecular Formula: C<sub>8</sub>H<sub>6</sub>ClNO<sub>4</sub>

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: C<sub>7</sub>H<sub>3</sub>Cl<sub>2</sub>NO<sub>3</sub>

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: C<sub>7</sub>H<sub>5</sub>ClN<sub>2</sub>O<sub>3</sub>

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: C<sub>7</sub>H<sub>3</sub>ClN<sub>2</sub>O<sub>2</sub>

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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Leonard, N.J. *et al.*, *J.O.C.*, 1946, **11**, 405, (*synth*)

Atkinson, R. *et al.*, *J.C.S.*, 1947, 232, (*synth*)

Goldstein, H. *et al.*, *Helv. Chim. Acta*, 1957, **40**, 369, (*synth*)

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