



>>Entry Name: 4-Chloro-3-nitrobenzoic acid, 9Cl, 8Cl

CAS Registry Number: 96-99-1

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. (EtOH)

Melting Point: Mp 183°

pKa Value: pK_a 3.34

Hazard & Toxicity: LD₅₀ (rat, orl) 3150 mg/kg

Aldrich: C6000-7

Fluka: 25450

Sigma: C9765

>>Derivative: Me ester

CAS Registry Number: 14719-83-6

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. (MeOH)

Melting Point: Mp 83°

Rare Chemicals Library: S70674-4

>>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 51°

Boiling Point: Bp₂₂ 170°

>>Derivative: Amide

CAS Registry Number: 16588-06-0

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 156°

Hazard & Toxicity: LD₅₀ (rat, orl) 2570 mg/kg

Rare Chemicals Library: S61396-7

>>Derivative: Anilide

Synonym(s): 4-Chloro-3-nitro-*N*-phenylbenzamide, 9Cl

CAS Registry Number: 41614-16-8

Molecular Formula: C₁₃H₉ClN₂O₃

Molecular Weight: 276.678

Accurate Mass: 276.03017

Percentage Composition: C 56.43%; H 3.28%; Cl 12.81%; N 10.12%; O 17.35%

Melting Point: Mp 133-136°

Rare Chemicals Library: S34441-9

Other: PB N07950