



>>Entry Name: 2-Chloro-4-nitrophenol

CAS Registry Number: 619-08-9

Structure by analogy with 2-Chloro-3-nitrophenol, [DXB82-O](#)

Molecular Formula: C₆H₄ClNO₃

Molecular Weight: 173.555

Accurate Mass: 172.987971

Percentage Composition: C 41.52%; H 2.32%; Cl 20.43%; N 8.07%; O 27.66%

Biological Source: Prod. by *Stephanospora caroticolor*

Biological Use/Importance: Fungicide

Physical Description: Needles (H₂O)

Melting Point: Mp 114°

pKa Value: pK_a 5.45 (25°)

Hazard & Toxicity: LD₅₀ (rat, orl) 900 mg/kg

Aldrich: C6120-8

>>Derivative: Ac

CAS Registry Number: 18855-84-0

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: Needles

Melting Point: Mp 63°

>>Derivative: Me ether

Synonym(s): 2-Chloro-1-methoxy-4-nitrobenzene. 2-Chloro-4-nitroanisole

CAS Registry Number: 4920-79-0

Molecular Formula: C₇H₆ClNO₃

Molecular Weight: 187.582

Accurate Mass: 187.003621

Percentage Composition: C 44.82%; H 3.22%; Cl 18.90%; N 7.47%; O 25.59%

Physical Description: Needles or prisms (MeOH)

Melting Point: Mp 98°

Hazard & Toxicity: Eye and skin irritant. LD₅₀ (rat, orl) 1180 mg/kg

>>Derivative: Et ether

Synonym(s): 2-Chloro-1-ethoxy-4-nitrobenzene. 2-Chloro-4-nitrophenetole

CAS Registry Number: 5493-71-0

Molecular Formula: C₈H₈ClNO₃

Molecular Weight: 201.609

Accurate Mass: 201.019271

Percentage Composition: C 47.66%; H 4.00%; Cl 17.58%; N 6.95%; O 23.81%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 82°

References:

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Poirier, J.-M. *et al.*, *Tetrahedron*, 1989, **45**, 1415-1422, (*synth, pmr*)

Makosza, M. *et al.*, *J.O.C.*, 1990, **55**, 4979-4981, (*synth*)

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