



>>Entry Name: 1-Chloro-3-nitrobenzene, 9Cl

Synonym(s): *m*-Chloronitrobenzene, 8Cl

CAS Registry Number: 121-73-3

Extra CAS Registry Numbers(s): 25167-93-5

Molecular Formula: C₆H₄ClNO₂

Molecular Weight: 157.556

Accurate Mass: 156.993056

Percentage Composition: C 45.74%; H 2.56%; Cl 22.50%; N 8.89%; O 20.31%

Physical Description: Pale-yellow prisms

Melting Point: Mp 46°

Boiling Point: Bp 235-236°

pKa Value: pK_a -12.15 (18°, H₂SO₄ aq.)

Hazard & Toxicity: Exposure by inhalation or skin absorption can cause methaemoglobinaemia leading to cyanosis. LD₅₀ (rat, orl) 470 mg/kg

Aldrich: 27002-4

Fluka: 25480

Rare Chemicals Library: S64314-9

References:

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Kurz, M. *et al.*, *Chem. Comm.*, 1976, 968, (*synth*)

Olah, G.A. *et al.*, *J.O.C.*, 1978, **43**, 4628, (*synth*)

Zuccarello, F. *et al.*, *Spectrochim. Acta A*, 1979, **35**, 223, (*uv*)

Schuster, I. *et al.*, *J.O.C.*, 1980, **45**, 284, (*N-15 nmr*)

Batts, B.D. *et al.*, *Org. Magn. Reson.*, 1980, **13**, 349, (*pmr*)

Harrison, A.G. *et al.*, *Org. Mass Spectrom.*, 1980, **15**, 286, (*ms*)

Brownlee, R.T.C. *et al.*, *Org. Magn. Reson.*, 1986, **24**, 862, (*cmr*)

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