



>>Entry Name: 1-Methyl-2,4-dinitrobenzene, 9CI

Synonym(s): 2,4-Dinitrotoluene, 8CI

CAS Registry Number: 121-14-2

Extra CAS Registry Numbers(s): 25321-14-6

Molecular Formula: $C_7H_6N_2O_4$

Molecular Weight: 182.135

Accurate Mass: 182.032758

Percentage Composition: C 46.16%; H 3.32%; N 15.38%; O 35.14%

Use/Importance: Widely used in prodn. of polyurethane foams, coatings, elastomers and explosives (usually as technical dinitrotoluene which cont. =75% this isomer)

Physical Description: Needles (CS_2)

Melting Point: Mp 71°

Boiling Point: Bp 300°

pKa Value: pK_a 17.12 (ethylenediamine aq.) pK_a -12.6 (oleum)

Hazard & Toxicity: Fl. p. 207°. Toxic by inhalation and skin absorption. Potentially explosive on prolonged heating or in the presence of base. Skin irritant and allergen. Can cause anaemia, methaemoglobinaemia, cyanosis and liver damage. LD₅₀ (rat, orl) 268 mg/kg. Exp. reprod. effects

Aldrich: 10139-7

Fluka: 42290

Rare Chemicals Library: S41855-2

Supelco: R43-0350

References:

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Priester, F. *et al.*, *Anal. Chem.*, 1960, **32**, 495, (ir)

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Mathias, A. *et al.*, *Anal. Chim. Acta*, 1966, **35**, 376, (pmr)

Coon, C.L. *et al.*, *J.O.C.*, 1973, **38**, 4243, (synth)

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