



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

Synonym(s): 2,5-Dinitrotoluene, 8CI

CAS Registry Number: 619-15-8

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%

Physical Description: Needles (EtOH)

Melting Point: Mp 52.5°

pKa Value: pK_a 3.54 (25°, ethylenediamine)

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 517 mg/kg. Exposure may cause methaemoglobinaemia

Rare Chemicals Library: S54909-6

References:

Page, H.J. *et al.*, *J.C.S.*, 1923, **123**, 3235, (*synth*)

Hodgson, H.H. *et al.*, *J.C.S.*, 1949, 1624, (*synth*)

Conduit, C.P., *J.C.S.*, 1959, 3273, (*ir, uv*)

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

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

Mori, M. *et al.*, *Chem. Pharm. Bull.*, 1984, **32**, 4070, (*metab, tox*)

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 2nd edn., Butterworths, 1979, 162

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