



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

Synonym(s): 3,4-Dinitrotoluene, 8CI

CAS Registry Number: 610-39-9

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%

Melting Point: Mp 61°

pKa Value: pK_a 3.18 (ethylenediamine)

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 177 mg/kg

Aldrich: 14812-1

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1369A, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1212A, (ir)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 1172C, (nmr)

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

Hodgson, H.H. *et al.*, *J.C.S.*, 1948, 1512, (synth)

Weygand, F. *et al.*, *Chem. Ber.*, 1950, **83**, 405, (synth)

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

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

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

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

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, DVH600

Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. *et al.*), J.B. Lippincott, 1988, 258