



>>Entry Name: 1-Methyl-3,5-dinitrobenzene, 9CI

Synonym(s): 3,5-Dinitrotoluene, 8CI

CAS Registry Number: 618-85-9

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%

Physical Description: Needles (AcOH)

Melting Point: Mp 93°

Hazard & Toxicity: LD₅₀ (rat, orl) 216 mg/kg

References:

Brady, O.L. *et al.*, *J.C.S.*, 1922, **121**, 528, (*synth*)

Morton, R.A. *et al.*, *J.C.S.*, 1934, 901, (*synth*)

Hodgson, H.H. *et al.*, *J.C.S.*, 1942, 748, (*synth*)

Smith, W.T. *et al.*, *J.A.C.S.*, 1953, **75**, 3602, (*synth*)

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

Beynon, J.H. *et al.*, *Ind. Chim. Belg.*, 1964, **29**, 311, (*ms*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DVH800

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