



>>Entry Name: **1,3-Dimethyl-5-nitrobenzene**, 9CI

Synonym(s): 5-Nitro-*m*-xylene, 8CI

CAS Registry Number: 99-12-7

Structure by analogy with 1,2-Dimethyl-3-nitrobenzene, [DVK05-Y](#)

Molecular Formula: C₈H₉NO₂

Molecular Weight: 151.165

Accurate Mass: 151.063329

Percentage Composition: C 63.57%; H 6.00%; N 9.27%; O 21.17%

Physical Description: Needles (EtOH)

Melting Point: Mp 75°

Boiling Point: Bp 251°

Aldrich: 13785-5

Rare Chemicals Library: S3638-3

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 753A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1372B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1213A, (*ir*)

Noyes, W.A., *Am. Chem. J.*, 1898, **20**, 789

Burgers, J. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1958, **77**, 491

Kinugasa, T. *et al.*, *Nippon Kagaku Zasshi*, 1962, **83**, 333

Nomura, Y. *et al.*, *Tet. Lett.*, 1968, 5585, (*nmr*)