



>>Entry Name: **2,6-Dimethyl-4-nitrophenol**

Synonym(s): 4-Nitro-2,6-xylenol

CAS Registry Number: 2423-71-4

Structure by analogy with 2,3-Dimethyl-4-nitrophenol, [BKB78-I](#)

Molecular Formula: $C_8H_9NO_3$

Molecular Weight: 167.164

Accurate Mass: 167.058244

Percentage Composition: C 57.48%; H 5.43%; N 8.38%; O 28.71%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 171°

pKa Value: pK_{a1} 7.07 (25°)

Aldrich: 13271-3

Fluka: 40890

>>Derivative: Me ether

Synonym(s): 2-Methoxy-1,3-dimethyl-5-nitrobenzene

CAS Registry Number: 14804-39-8

Molecular Formula: $C_9H_{11}NO_3$

Molecular Weight: 181.191

Accurate Mass: 181.073894

Percentage Composition: C 59.66%; H 6.12%; N 7.73%; O 26.49%

Physical Description: Pale-yellow needles (EtOH)

Melting Point: Mp 92°

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 761B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1374D, (*ir*)

Fischer, A., *J.C.S.(B)*, 1966, 782, (*synth*)

Fujio, M. *et al.*, *Bull. Chem. Soc. Jpn.*, 1975, **48**, 2127, (*synth*)

Gaude, D. *et al.*, *Synth. Commun.*, 1986, **16**, 63, (*synth*)