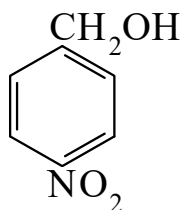




>>Entry Name: 4-Nitrobenzyl alcohol

Synonym(s): 4-Nitrobenzenemethanol, 9CI. 1-Hydroxymethyl-4-nitrobenzene. α -Hydroxy-4-nitrotoluene



CAS Registry Number: 619-73-8

Molecular Formula: C₇H₇NO₃

Molecular Weight: 153.137

Accurate Mass: 153.042594

Percentage Composition: C 54.90%; H 4.61%; N 9.15%; O 31.34%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 92-93°

Boiling Point: Bp₁₂ 185°

Aldrich: N1282-1

Fluka: 73160

Rare Chemicals Library: S3622-7

Sigma: N6251

>>Derivative: O-Benzoyl

CAS Registry Number: 4457-41-4

Molecular Formula: C₁₄H₁₁NO₄

Molecular Weight: 257.245

Accurate Mass: 257.068809

Percentage Composition: C 65.37%; H 4.31%; N 5.44%; O 24.88%

Melting Point: Mp 94-95°

Rare Chemicals Library: S91915-2

>>Derivative: 4-Methylbenzenesulfonyl

CAS Registry Number: 4450-68-4

Use/Importance: Protecting reagent for peptides. Uv labelling reagent for carboxylic acids

Melting Point: Mp 103°

>>Derivative: Ph ether

Synonym(s): 1-Nitro-4-(phenoxy)methylbenzene. 4-Nitrobenzyl phenyl ether

CAS Registry Number: 3048-12-2

Molecular Formula: C₁₃H₁₁NO₃

Molecular Weight: 229.235

Accurate Mass: 229.073894

Percentage Composition: C 68.11%; H 4.84%; N 6.11%; O 20.94%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 89-91°

Rare Chemicals Library: S64624-5

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 697C, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1341D, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1193A, (*ir*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 737
Koizumi, T. *et al.*, *Chem. Pharm. Bull.*, 1973, **21**, 312, (*synth*)
Lane, C.F. *et al.*, *J.O.C.*, 1974, **39**, 3052, (*synth*)
Maslak, P. *et al.*, *J.A.C.S.*, 1986, **108**, 2628, (*deriv, synth, pmr, ms*)
Funazo, K. *et al.*, *J. Chromatogr.*, 1989, **481**, 211, (*use, tosylate*)