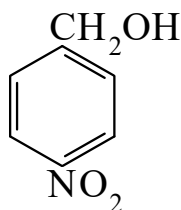




**>>Entry Name: 4-Nitrobenzyl alcohol**

**Synonym(s):** 4-Nitrobenzenemethanol, 9CI. 1-Hydroxymethyl-4-nitrobenzene.  $\alpha$ -Hydroxy-4-nitrotoluene



**CAS Registry Number:** 619-73-8

**Molecular Formula:** C<sub>7</sub>H<sub>7</sub>NO<sub>3</sub>

**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. (H<sub>2</sub>O)

**Melting Point:** Mp 92-93°

**Boiling Point:** Bp<sub>12</sub> 185°

**Aldrich:** N1282-1

**Fluka:** 73160

**Rare Chemicals Library:** S3622-7

**Sigma:** N6251

**>>Derivative: O-Benzoyl**

**CAS Registry Number:** 4457-41-4

**Molecular Formula:** C<sub>14</sub>H<sub>11</sub>NO<sub>4</sub>

**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:** C<sub>13</sub>H<sub>11</sub>NO<sub>3</sub>

**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*)