



>>Entry Name: 4-Pentyn-1-ol, 9CI

CAS Registry Number: 5390-04-5

HC#CCH2CH2CH2OH

Molecular Formula: C_5H_8O

Molecular Weight: 84.118

Accurate Mass: 84.057515

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Boiling Point: Bp 154°

Aldrich: 30248-1

Fluka: 77053

>>Derivative: Methanesulfonyl

Molecular Formula: $C_6H_{10}O_3S$

Molecular Weight: 162.209

Accurate Mass: 162.035065

Percentage Composition: C 44.43%; H 6.21%; O 29.59%; S 19.77%

Physical Description: Oil

Boiling Point: Bp_{0.45} 85-90° (bath)

>>Derivative: 1-Naphthylurethane

Molecular Formula: $C_{16}H_{15}NO_2$

Molecular Weight: 253.3

Percentage Composition: C 75.87%; H 5.97%; N 5.53%; O 12.63%

Physical Description: Cryst. (petrol)

Melting Point: Mp 79-80°

>>Derivative: Tetrahydropyranyl

Molecular Formula: $C_{10}H_{16}O_2$

Molecular Weight: 168.235

Accurate Mass: 168.11503

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Physical Description: Oil

Boiling Point: Bp_{0.3} 40-41°

>>Derivative: Et ether

Synonym(s): 5-Ethoxy-1-pentyne

Molecular Formula: $C_7H_{12}O$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Boiling Point: Bp₂₅ 38°

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **3**, 511A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1586D, (*ir*)

Eglinton, G. *et al.*, *J.C.S.*, 1952, 2873

Colonge, J. *et al.*, *Bull. Soc. Chim. Fr.*, 1954, 797, (*synth*)

Org. Synth., Coll. Vol., 4, 1963, 755, (*synth*)

Schaub, B. *et al.*, *Helv. Chim. Acta*, 1975, **58**, 556, (*synth*, *pmr*)

Kita, Y. *et al.*, *J.O.C.*, 1991, **56**, 119, (*synth*, *ir*, *pmr*)