



>>Entry Name: 2-Octyn-1-ol, 9CI
Synonym(s): Pentylpropargyl alcohol

CAS Registry Number: 20739-58-6
H3C(CH2)4C#CCCH2OH

Molecular Formula: C₈H₁₄O
Molecular Weight: 126.198
Accurate Mass: 126.104465
Percentage Composition: C 76.14%; H 11.18%; O 12.68%
Physical Description: Liq.
Boiling Point: Bp₈ 90°
Density: d₄¹⁷ 0.884
Refractive Index: n_D¹⁷ 1.4585

Fluka: 74976
Rare Chemicals Library: S88495-2

>>Derivative: Ac

CAS Registry Number: 16491-64-8
Molecular Formula: C₁₀H₁₆O₂
Molecular Weight: 168.235
Accurate Mass: 168.11503
Percentage Composition: C 71.39%; H 9.59%; O 19.02%
Boiling Point: Bp₆ 79-81°

References:

- Sood, R. *et al.*, *Tet. Lett.*, 1974, 423-425, (*synth*)
Rickards, G. *et al.*, *J.O.C.*, 1978, **43**, 3607-3609, (*synth, ir, pmr, ms*)
Porter, N.A. *et al.*, *J.O.C.*, 1985, **50**, 2252-2258, (*synth, pmr*)
Kanakam, C.C. *et al.*, *J.C.S. Perkin I*, 1989, 1907-1913, (*synth, ir, pmr*)
Zhengming, L. *et al.*, *Synth. Commun.*, 1989, **19**, 91-96, (*synth, pmr*)
Crombie, L. *et al.*, *J.C.S. Perkin I*, 1991, 567-575, (*synth, ir, pmr*)
Poleschner, H. *et al.*, *Magn. Reson. Chem.*, 1995, **33**, 917-921, (*cmr*)
Zwierzak, A. *et al.*, *Synth. Commun.*, 1996, **26**, 3593-3600, (*synth, ir, pmr*)
Bruckner, R. *et al.*, *Chem. Eur. J.*, 1998, **4**, 2342-2352, (*synth, ir, pmr*)
Capon, R.J. *et al.*, *J.O.C.*, 1998, **63**, 75-83, (*synth, ir, pmr, cmr, ms*)
Havranek, M. *et al.*, *Synthesis*, 1998, 1264-1268, (*synth*)