



>>Entry Name: 3-Hexene-1,6-diol, 9CI

CAS Registry Number: 67077-43-4

Related CAS Registry Numbers(s): 57042-14-5 57086-89-2 69182-63-4
HOCH2CH2CH=CHCH2CH2OH

Molecular Formula: $C_6H_{12}O_2$

Molecular Weight: 116.16

Accurate Mass: 116.08373

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

>>Variant: (E)-form

CAS Registry Number: 71655-17-9

Molecular Formula: $C_6H_{12}O_2$

Molecular Weight: 116.16

Accurate Mass: 116.08373

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Physical Description: Viscous, hygroscopic liq.

Boiling Point: $B_{p0.3}$ 88-90°

Refractive Index: n_D^{18} 1.4747

>>Derivative: Bisphenylurethane

Physical Description: Plates (toluene)

Melting Point: Mp 161-162°

>>Variant: (Z)-form

CAS Registry Number: 72530-33-7

Molecular Formula: $C_6H_{12}O_2$

Molecular Weight: 116.16

Accurate Mass: 116.08373

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Physical Description: Viscous, hygroscopic liq.

Boiling Point: $B_{p0.3}$ 86-87°

Refractive Index: n_D^{15} 1.4750

>>Derivative: Bisphenylurethane

Physical Description: Needles (petrol)

Melting Point: Mp 107-108°

References:

- Raphael, R.A. *et al.*, *J.C.S.*, 1952, 3875, (*synth, derivs*)
Vukov, V. *et al.*, *Can. J. Chem.*, 1975, **53**, 1367, (*synth*)
Levisalles, J. *et al.*, *Tetrahedron*, 1980, **36**, 3181, (*synth, ir, Raman, ms*)
Majumdar, K.C. *et al.*, *Indian J. Chem., Sect. B*, 1984, **23**, 303, (*synth*)
Allan, R.D. *et al.*, *Aust. J. Chem.*, 1985, **38**, 1651, (*synth, pmr*)
Gassman, P.G. *et al.*, *J.A.C.S.*, 1989, **111**, 2652, (*synth, ir, pmr, cmr*)
Cantin, M. *et al.*, *Can. J. Chem.*, 1990, **68**, 2144, (*synth, pmr*)
Eya, B.K. *et al.*, *Tetrahedron*, 1990, **46**, 2695, (*synth*)