



>>Entry Name: 2,4-Hexadiyne-1,6-diol, 9CI

CAS Registry Number: 3031-68-3

HOCH₂C≡CC≡CCH₂OH

Molecular Formula: C₆H₆O₂

Molecular Weight: 110.112

Accurate Mass: 110.03678

Percentage Composition: C 65.45%; H 5.49%; O 29.06%

Use/Importance: Used in polymerisation studies

Physical Description: Tan solid or platelets (H₂O)

Melting Point: Mp 109-112°

Fluka: 52490

Rare Chemicals Library: S70462-8

>>Derivative: Bis(4-methylbenzenesulfonyl)

CAS Registry Number: 32527-15-4

Physical Description: Plates (MeOH)

Melting Point: Mp 96°

Other Data: Turns pink on exp. to light. Mp variable due to polym. on heating

>>Derivative: Di-Me ether

Synonym(s): 1,6-Dimethoxy-2,4-hexadiyne

CAS Registry Number: 20726-67-4

Molecular Formula: C₈H₁₀O₂

Molecular Weight: 138.166

Accurate Mass: 138.06808

Percentage Composition: C 69.55%; H 7.29%; O 23.16%

Physical Description: Yellow liq.

Boiling Point: Bp_{0.5} 50°

Refractive Index: n_D²⁰ 1.5000

Other Data: Turns brown on standing

References:

- Lespieau, M.R., *Ann. Chim. (Paris)*, 1897, **11**, 232, (*synth*)
Armitage, J.B. *et al.*, *J.C.S.*, 1952, 1998; 2005, (*synth, uv, derivs*)
Haedicke, E., *Angew. Chem., Int. Ed.*, 1971, **10**, 940, (*cryst struct*)
Schwarz, H., *Org. Mass Spectrom.*, 1976, **11**, 313, (*uv*)
Hearn, M.T.W., *Org. Magn. Reson.*, 1977, **9**, 141, (*cmr*)
Patel, E.N., *J. Polym. Sci., Polym. Phys. Ed.*, 1979, **17**, 159, (*ditosyl*)
Wityak, J. *et al.*, *Synth. Commun.*, 1991, **21**, 977, (*synth*)
Cai, C. *et al.*, *Helv. Chim. Acta*, 1995, **78**, 2053, (*synth, ir, cmr, ms, di-Me ether*)
Bierer, D.E. *et al.*, *J. Med. Chem.*, 1995, **38**, 2628, (*synth, pmr, cmr*)