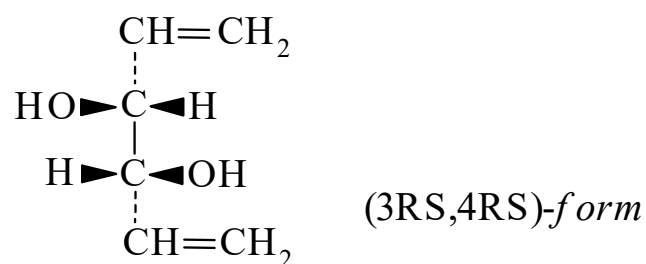




>>Entry Name: 1,5-Hexadiene-3,4-diol, 9CI

Synonym(s): Divinylethylene glycol. 1,2-Divinylglycol



CAS Registry Number: 1069-23-4

Related CAS Registry Numbers(s): 58208-04-1

Molecular Formula: C₆H₁₀O₂

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Use/Importance: Used in the synth. of bioadhesive cross-linked acrylic polymers

Hazard & Toxicity: LD₅₀ (rat, orl) 1620 mg/kg; LD₅₀ (rbt, skn) 400 mg/kg

Aldrich: 37644-2

Rare Chemicals Library: S37521-7

>>Variant: (3RS,4RS)-form

Synonym(s): (±)-form

CAS Registry Number: 19700-97-1

Molecular Formula: C₆H₁₀O₂

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Melting Point: Mp 21.7°

Boiling Point: Bp₈ 90.5°

>>Variant: (3RS,4SR)-form

Synonym(s): *meso*-form

CAS Registry Number: 19700-96-0

Molecular Formula: C₆H₁₀O₂

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Physical Description: Cryst. (petrol)

Melting Point: Mp 88°

>>Derivative: Di-Et ether

Synonym(s): 3,4-Diethoxy-1,5-hexadiene

Molecular Formula: C₁₀H₁₈O₂

Molecular Weight: 170.251

Accurate Mass: 170.13068

Percentage Composition: C 70.55%; H 10.66%; O 18.80%

Boiling Point: Bp 224-226°. Bp₁₀ 111-113°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 223A, (*nmr*)

Young, W.G. *et al.*, *J.A.C.S.*, 1943, **65**, 1245, (*synth*)

Braun, R.A., *J.O.C.*, 1963, **28**, 1383, (*synth*)

Wiemann, J. *et al.*, *Bull. Soc. Chim. Fr.*, 1967, 3293, (*synth*)

Galaj, S. *et al.*, *Bull. Soc. Chim. Fr.*, 1972, 3979, (*synth*)

Ching, H.S. *et al.*, *J. Pharm. Sci.*, 1985, **74**, 399, (*use*)

Rao, A.V.R. *et al.*, *Tet. Lett.*, 1987, **28**, 2183, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DMU000