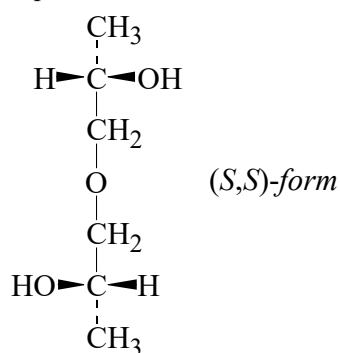




>>Entry Name: 1,1'-Oxybis-2-propanol

Synonym(s): Dipropylene glycol. Bis(2-hydroxypropyl) ether. 4-Oxaheptane-2,6-diol



CAS Registry Number: 110-98-5

Related CAS Registry Numbers(s): 35884-42-5

Molecular Formula: C₆H₁₄O₃

Molecular Weight: 134.175

Accurate Mass: 134.094295

Percentage Composition: C 53.71%; H 10.52%; O 35.77%

Use/Importance: Intermed. in prepn. of macrocyclic ethers

Melting Point: Mp 46-48°

Boiling Point: Bp 228-230°. Bp₁₀ 113°

Density: d₄⁶⁰ 0.99

Refractive Index: n_D⁶⁰ 1.4284

Aldrich: D21555-4

>>Variant: (S,S)-form

Synonym(s): (+)-*threo*-form

CAS Registry Number: 61217-63-8

Molecular Formula: C₆H₁₄O₃

Molecular Weight: 134.175

Accurate Mass: 134.094295

Percentage Composition: C 53.71%; H 10.52%; O 35.77%

Physical Description: Oil

Optical Rotation: [α]_D²⁰ +52 (c, 2.3 in CHCl₃). [α]_D²⁵ +49.7 (c, 3.3 in CHCl₃) (>=98% ee)

>>Derivative: Bis-4-methylbenzenesulfonate

Molecular Formula: C₂₀H₂₆O₇S₂

Molecular Weight: 442.553

Accurate Mass: 442.111995

Percentage Composition: C 54.28%; H 5.92%; O 25.31%; S 14.49%

Physical Description: Oil

Optical Rotation: [α]_D²⁰ -9.9 (c, 11.3 in CHCl₃)

>>Variant: (RS,RS)-form

Synonym(s): (±)-form

CAS Registry Number: 55716-55-7

Molecular Formula: C₆H₁₄O₃

Molecular Weight: 134.175

Accurate Mass: 134.094295

Percentage Composition: C 53.71%; H 10.52%; O 35.77%

Physical Description: Viscous liq.

Boiling Point: Bp 218-221°

>>Derivative: Bis-4-methylbenzenesulfonate

CAS Registry Number: 55716-57-9

Molecular Formula: C₂₀H₂₆O₇S₂

Molecular Weight: 442.553

Accurate Mass: 442.111995

Percentage Composition: C 54.28%; H 5.92%; O 25.31%; S 14.49%

Physical Description: Prisms (MeOH)

Melting Point: Mp 47-50°