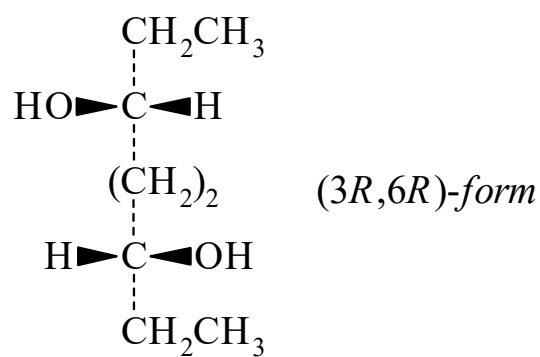




>>Entry Name: 3,6-Octanediol



CAS Registry Number: 24434-09-1

Related CAS Registry Numbers(s): 151124-02-6

Extra CAS Registry Numbers(s): 26762-67-4

Molecular Formula: C₈H₁₈O₂

Molecular Weight: 146.229

Accurate Mass: 146.13068

Percentage Composition: C 65.71%; H 12.41%; O 21.88%

>>Variant: (3*R*,6*R*)-form

CAS Registry Number: 129619-37-0

Molecular Formula: C₈H₁₈O₂

Molecular Weight: 146.229

Accurate Mass: 146.13068

Percentage Composition: C 65.71%; H 12.41%; O 21.88%

Physical Description: Cryst. solid (Et₂O)

Melting Point: Mp 51-52°

Optical Rotation: [α]_D²⁵ -22.8 (c, 1 in CHCl₃) (>99% ee)

>>Variant: (3*S*,6*S*)-form

CAS Registry Number: 136705-66-3

Molecular Formula: C₈H₁₈O₂

Molecular Weight: 146.229

Accurate Mass: 146.13068

Percentage Composition: C 65.71%; H 12.41%; O 21.88%

Optical Rotation: [α]_D²⁵ +22.8 (c, 1 in CHCl₃)

>>Derivative: Cyclic sulfate

Synonym(s): 4,7-Diethyl-1,3,2-dioxathiepane 2,2-dioxide, 9CI

CAS Registry Number: 136705-67-4

Molecular Formula: C₈H₁₆O₄S

Molecular Weight: 208.278

Accurate Mass: 208.07693

Percentage Composition: C 46.13%; H 7.74%; O 30.73%; S 15.40%

Physical Description: Cryst. (Et₂O/hexane)

Melting Point: Mp 79.5-80.5°

Optical Rotation: [α]_D²⁵ +28.6 (c, 1 in CHCl₃)

References:

Sudweeks, W.H. *et al.*, *J.O.C.*, 1975, **40**, 1131, (*synth*)

Burk, M.J. *et al.*, *Tetrahedron: Asymmetry*, 1991, **2**, 569, (*synth, pmr, cmr*)

Burk, M.J. *et al.*, *J.A.C.S.*, 1993, **115**, 10125, (*sulfate, synth, pmr, cmr*)