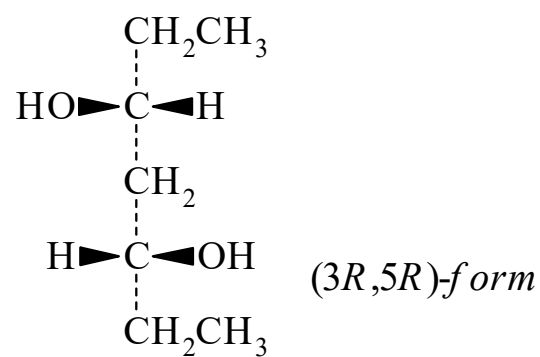




>>Entry Name: 3,5-Heptanediol, 9CI



CAS Registry Number: 86632-40-8

Molecular Formula: C₇H₁₆O₂

Molecular Weight: 132.202

Accurate Mass: 132.11503

Percentage Composition: C 63.60%; H 12.20%; O 24.20%

>>Variant: (3R,5R)-form

CAS Registry Number: 77291-90-8

Molecular Formula: C₇H₁₆O₂

Molecular Weight: 132.202

Accurate Mass: 132.11503

Percentage Composition: C 63.60%; H 12.20%; O 24.20%

Physical Description: Cryst.

Melting Point: Mp 52-53°

Boiling Point: Bp₁₂ 110°

Optical Rotation: [α]_D²⁰ -39.1 (c, 10 in EtOH)

>>Variant: (3S,5S)-form

CAS Registry Number: 129212-21-1

Molecular Formula: C₇H₁₆O₂

Molecular Weight: 132.202

Accurate Mass: 132.11503

Percentage Composition: C 63.60%; H 12.20%; O 24.20%

Physical Description: Cryst.

Melting Point: Mp 52-54°

Optical Rotation: [α]_D²⁵ +25 (c, 1 in CHCl₃)

>>Variant: (±)-form

Molecular Formula: C₇H₁₆O₂

Molecular Weight: 132.202

Accurate Mass: 132.11503

Percentage Composition: C 63.60%; H 12.20%; O 24.20%

Physical Description: Oil

Boiling Point: Bp₂₄ 127-130°

Other Data: Mixt. of diastereoisomers

References:

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Yang, G.K. *et al.*, *J.A.C.S.*, 1983, **105**, 6045-6052, (*synth*, *pmr*)

Rychnovsky, S.D. *et al.*, *J.O.C.*, 1991, **56**, 5161-5169, (*synth*, *ir*, *pmr*, *cmr*)

Marinetti, A. *et al.*, *Chem. Eur. J.*, 1999, **5**, 1160-1165, (*synth*, *pmr*)