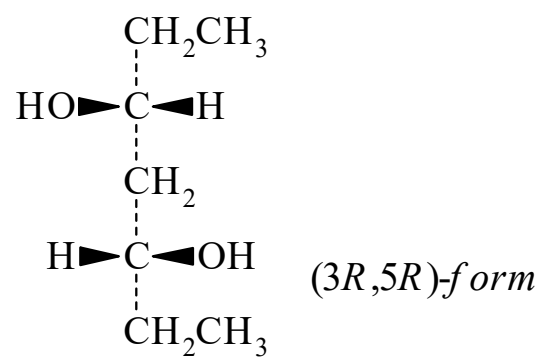




>>Entry Name: 3,5-Heptanediol, 9CI



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: (3*R*,5*R*)-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: (3*S*,5*S*)-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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