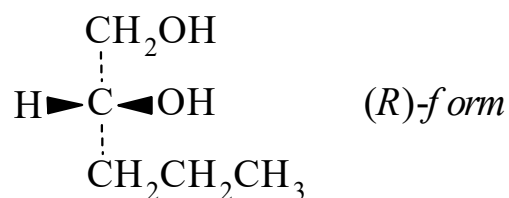




>>Entry Name: 1,2-Pentanediol, 9CI



CAS Registry Number: 5343-92-0

Related CAS Registry Numbers(s): 29117-54-2

Molecular Formula: C₅H₁₂O₂

Molecular Weight: 104.149

Accurate Mass: 104.08373

Percentage Composition: C 57.66%; H 11.61%; O 30.72%

Aldrich: 26028-2

Fluka: 76891

>>Variant: (R)-form

CAS Registry Number: 108340-61-0

Molecular Formula: C₅H₁₂O₂

Molecular Weight: 104.149

Accurate Mass: 104.08373

Percentage Composition: C 57.66%; H 11.61%; O 30.72%

Boiling Point: Bp₁₃ 98-102°

Optical Rotation: [α]_D²⁰ +0.95

>>Derivative: Bisphenylurethane

Molecular Formula: C₁₉H₂₂N₂O₄

Molecular Weight: 342.394

Accurate Mass: 342.157958

Percentage Composition: C 66.65%; H 6.48%; N 8.18%; O 18.69%

Melting Point: Mp 97-98°

>>Variant: (±)-form

CAS Registry Number: 91049-43-3

Molecular Formula: C₅H₁₂O₂

Molecular Weight: 104.149

Accurate Mass: 104.08373

Percentage Composition: C 57.66%; H 11.61%; O 30.72%

Physical Description: Oil

Boiling Point: Bp 210.5-211.5°. Bp_{0.3} 78-80°

Density: d₂₀²⁰ 0.971

Refractive Index: n_D²⁰ 1.4400

>>Derivative: Di-Ac

CAS Registry Number: 134172-59-1

Molecular Formula: C₉H₁₆O₄

Molecular Weight: 188.223

Accurate Mass: 188.10486

Percentage Composition: C 57.43%; H 8.57%; O 34.00%

Boiling Point: Bp 219-220°. Bp₂ 103-104°

References:

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