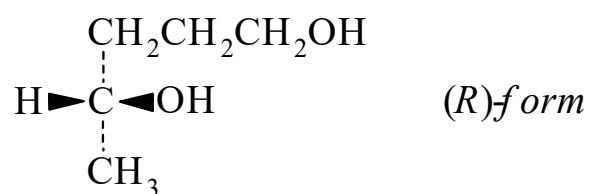




>>Entry Name: 1,4-Pentanediol, 9CI



CAS Registry Number: 626-95-9

Related CAS Registry Numbers(s): 24347-57-7

Molecular Formula: C₅H₁₂O₂

Molecular Weight: 104.149

Accurate Mass: 104.08373

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

Aldrich: 19418-2

>>Variant: (R)-form

CAS Registry Number: 56718-04-8

Molecular Formula: C₅H₁₂O₂

Molecular Weight: 104.149

Accurate Mass: 104.08373

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

Boiling Point: Bp_{1.5} 95-96°

Optical Rotation: [α]_D²² -4.9 (EtOH)

Other Data: Clearly optically impure (cf. S-isomer preparation below)

>>Derivative: Bisphenylurethane

Melting Point: Mp 131-133°

>>Variant: (S)-form

Molecular Formula: C₅H₁₂O₂

Molecular Weight: 104.149

Accurate Mass: 104.08373

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

Physical Description: Viscous oil

Optical Rotation: [α]_D²⁰ +19.3 (c, 1.0 in CHCl₃)

>>Variant: (±)-form

Molecular Formula: C₅H₁₂O₂

Molecular Weight: 104.149

Accurate Mass: 104.08373

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

Boiling Point: Bp₇₁₃ 219-220°. Bp₁₀ 124-126°

Solubility: Sol. H₂O, insol. petrol

Density: d₀⁰ 1

Refractive Index: n_D¹⁷ 1.4439

>>Derivative: Di-Ac

CAS Registry Number: 32864-71-4

Molecular Formula: C₉H₁₆O₄

Molecular Weight: 188.223

Accurate Mass: 188.10486

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

Boiling Point: Bp₁₃ 107-110°

>>Derivative: Bis-1-naphthylurethane

Melting Point: Mp 128-129.5°

References: