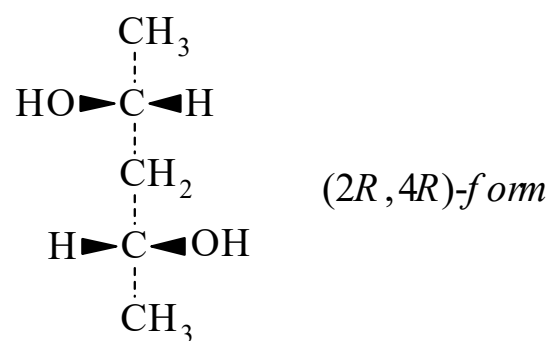




>>Entry Name: 2,4-Pentanediol, 9CI



CAS Registry Number: 625-69-4

Molecular Formula: C₅H₁₂O₂

Molecular Weight: 104.149

Accurate Mass: 104.08373

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

Hazard & Toxicity: Eye irritant

Aldrich: 15601-9

Fluka: 76900

>>Variant: (2*R*,4*R*)-form

CAS Registry Number: 42075-32-1

Molecular Formula: C₅H₁₂O₂

Molecular Weight: 104.149

Accurate Mass: 104.08373

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

Melting Point: Mp 50.5°

Boiling Point: Bp₁₉ 111-113°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -53.7$ (c, 10 in EtOH)

Aldrich: 24317-5

Fluka: 76897

Sigma: P4152

>>Derivative: Di-Ac

CAS Registry Number: 72345-24-5

Molecular Formula: C₉H₁₆O₄

Molecular Weight: 188.223

Accurate Mass: 188.10486

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

Optical Rotation: $[\alpha]_{\text{D}}^{20} -40.5$ (c, 10 in EtOH)

>>Variant: (2*R*,4*S*)-form

Molecular Formula: C₅H₁₂O₂

Molecular Weight: 104.149

Accurate Mass: 104.08373

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

Other Data: *meso*-Diastereoisomer found naturally as chiral monosubstituted glycosides

>>Derivative: 2-*O*-β-D-Glucopyranoside

Molecular Formula: C₁₁H₂₂O₇

Molecular Weight: 266.291

Accurate Mass: 266.136555

Percentage Composition: C 49.62%; H 8.33%; O 42.06%

Biological Source: Constit. of *Crescentia cujete*

Physical Description: Oil

Optical Rotation: $[\alpha]_{\text{D}} -33$ (c, 1.3 in MeOH)