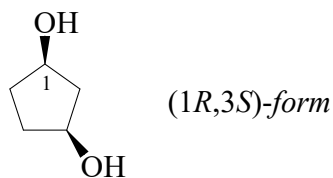




>>Entry Name: 1,3-Cyclopentanediol, 9CI

Synonym(s): 1,3-Dihydroxycyclopentane



CAS Registry Number: 59719-74-3

Related CAS Registry Numbers(s): 38551-63-2

Molecular Formula: C₅H₁₀O₂

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

General Statement: The original assignment of configs. (Owen, 1952) was incorrect

Aldrich: 19280-5

>>Variant: (1*R*,3*S*)-form

Molecular Formula: C₅H₁₀O₂

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

Other Data: The (*R,S*)-form is a *meso* diastereoisomer but is known as chiral monosubstituted derivs

>>Derivative: 1-Ac

CAS Registry Number: 149342-57-4

Molecular Formula: C₇H₁₂O₃

Molecular Weight: 144.17

Accurate Mass: 144.078645

Percentage Composition: C 58.32%; H 8.39%; O 33.29%

Boiling Point: Bp₁ 60-80° (kugelrohr)

Optical Rotation: [α]_D²⁰ -5.43 (c, 1.03 in MeOH)

>>Derivative: 1-Ac, 3-methanesulfonyl

CAS Registry Number: 149287-86-5

Molecular Formula: C₈H₁₄O₅S

Molecular Weight: 222.262

Accurate Mass: 222.056195

Percentage Composition: C 43.23%; H 6.35%; O 35.99%; S 14.43%

Physical Description: Yellow oil

>>Variant: (1*S*,3*R*)-form

Molecular Formula: C₅H₁₀O₂

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

>>Derivative: 1-Ac

CAS Registry Number: 149342-58-5

Molecular Formula: C₇H₁₂O₃

Molecular Weight: 144.17

Accurate Mass: 144.078645

Percentage Composition: C 58.32%; H 8.39%; O 33.29%

Optical Rotation: [α]_D²³ +5.8 (c, 0.012 in CHCl₃)

>>Derivative: 1-Ac, 3-methanesulfonyl

CAS Registry Number: 149342-59-6

Physical Description: Yellow oil