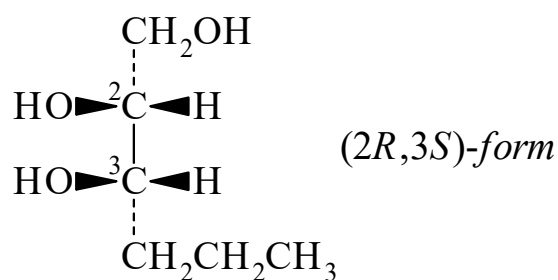




>>Entry Name: 1,2,3-Hexanetriol, 9CI

Synonym(s): 1-Propylglycerol. 4,5,6-Trideoxyhexitol



CAS Registry Number: 90325-47-6

Related CAS Registry Numbers(s): 64446-63-5 83134-92-3

Extra CAS Registry Numbers(s): 25323-24-4

Molecular Formula: $\text{C}_6\text{H}_{14}\text{O}_3$

Molecular Weight: 134.175

Accurate Mass: 134.094295

Percentage Composition: C 53.71%; H 10.52%; O 35.77%

Aldrich: 37497-0

>>Variant: (2R,3S)-form

Synonym(s): D-erythro-form

CAS Registry Number: 95839-99-9

Molecular Formula: $\text{C}_6\text{H}_{14}\text{O}_3$

Molecular Weight: 134.175

Accurate Mass: 134.094295

Percentage Composition: C 53.71%; H 10.52%; O 35.77%

>>Derivative: Tri-Ac

CAS Registry Number: 96751-56-3

Molecular Formula: $\text{C}_{12}\text{H}_{20}\text{O}_6$

Molecular Weight: 260.286

Accurate Mass: 260.12599

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

Physical Description: Oil

Optical Rotation: $[\alpha]_{\text{D}}^{20} -1.8$ (c, 2.4 in CHCl_3)

>>Variant: (2S,3R)-form

Synonym(s): L-erythro-form

CAS Registry Number: 130855-55-9

Molecular Formula: $\text{C}_6\text{H}_{14}\text{O}_3$

Molecular Weight: 134.175

Accurate Mass: 134.094295

Percentage Composition: C 53.71%; H 10.52%; O 35.77%

Melting Point: Mp 82°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -8.9$ (c, 2.2 in H_2O)

>>Derivative: 3-Benzoyl

CAS Registry Number: 142204-60-2

Molecular Formula: $\text{C}_{13}\text{H}_{18}\text{O}_4$

Molecular Weight: 238.283

Accurate Mass: 238.12051

Percentage Composition: C 65.53%; H 7.61%; O 26.86%

Optical Rotation: $[\alpha]_{\text{D}}^{25} +24.1$ (c, 1.52 in CHCl_3)

>>Derivative: Tri-Ac

CAS Registry Number: 99666-14-5

Physical Description: Syrup

Optical Rotation: $[\alpha]_{\text{D}}^{20} -1.8$ (c, 2.4 in CHCl_3)