



>>Variant: (S)-form

Molecular Formula: C₆H₁₂O₄

Molecular Weight: 148.158

Accurate Mass: 148.07356

Percentage Composition: C 48.64%; H 8.16%; O 43.20%

Physical Description: Oil

>>Derivative: Nitrile

Synonym(s): 4-Cyano-3-methyl-1,3-butanediol. Mevalononitrile. 3,5-Dihydroxy-3-methylpentanenitrile

CAS Registry Number: 176589-60-9

Molecular Formula: C₆H₁₁NO₂

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Physical Description: Viscous oil

Optical Rotation: [α]_D²⁴ +1.62 (c, 1.63 in CHCl₃) (93% ee)

>>Derivative: δ -Lactone

CAS Registry Number: 19022-60-7

Molecular Formula: C₆H₁₀O₃

Molecular Weight: 130.143

Accurate Mass: 130.062995

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

Physical Description: Cryst.

Melting Point: Mp 28°

Optical Rotation: [α]_D²⁶ +22.8 (c, 10 in EtOH)

>>Variant: (±)-form

CAS Registry Number: 690-72-2

Molecular Formula: C₆H₁₂O₄

Molecular Weight: 148.158

Accurate Mass: 148.07356

Percentage Composition: C 48.64%; H 8.16%; O 43.20%

>>Derivative: δ -Lactone

CAS Registry Number: 674-26-0

Molecular Formula: C₆H₁₀O₃

Molecular Weight: 130.143

Accurate Mass: 130.062995

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

Melting Point: Mp 27-28°

Boiling Point: Bp_{0.1} 110°

Fluka: 69761

Sigma: M9627

References: