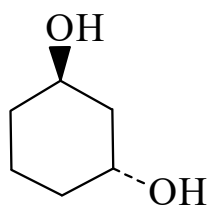




>>Entry Name: 1,3-Cyclohexanediol, 9CI
Synonym(s): Hexahydroresorcinol. Resorcitol



(1*R*,3*R*)-form

CAS Registry Number: 504-01-8
Related CAS Registry Numbers(s): 2867-32-5 103668-41-3

Molecular Formula: C₆H₁₂O₂
Molecular Weight: 116.16
Accurate Mass: 116.08373
Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Aldrich: C10110-9
Rare Chemicals Library: S44131-7

>>Variant: (1*R*,3*R*)-form
Synonym(s): (±)-*trans*-form

CAS Registry Number: 5515-64-0
Molecular Formula: C₆H₁₂O₂
Molecular Weight: 116.16
Accurate Mass: 116.08373
Percentage Composition: C 62.04%; H 10.41%; O 27.55%
Melting Point: Mp 117°

>>Derivative: Di-Ac

CAS Registry Number: 26688-53-9
Molecular Formula: C₁₀H₁₆O₄
Molecular Weight: 200.234
Accurate Mass: 200.10486
Percentage Composition: C 59.98%; H 8.05%; O 31.96%
Boiling Point: Bp_{0.4} 95°

>>Derivative: Dibenzoyl

CAS Registry Number: 79455-21-3
Molecular Formula: C₂₀H₂₀O₄
Molecular Weight: 324.376
Accurate Mass: 324.13616
Percentage Composition: C 74.06%; H 6.21%; O 19.73%
Physical Description: Cryst. (AcOH, EtOH or petrol)
Melting Point: Mp 123.5°

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

CAS Registry Number: 823-18-7
Molecular Formula: C₆H₁₂O₂
Molecular Weight: 116.16
Accurate Mass: 116.08373
Percentage Composition: C 62.04%; H 10.41%; O 27.55%
Physical Description: Cryst. (EtOAc or Me₂CO)
Solubility: Sol. H₂O, EtOH, spar. sol. Et₂O, petrol, C₆H₆

>>Derivative: Dibenzoyl

CAS Registry Number: 20134-00-3
Physical Description: Cryst. (MeOH or petrol)
Melting Point: Mp 65.5°

References: