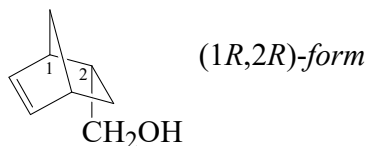




>>Entry Name: Bicyclo[2.2.1]hept-5-ene-2-methanol, 9CI

Synonym(s): 5-Norbornene-2-methanol, 8CI. 2-(Hydroxymethyl)bicyclo[2.2.1]hept-5-ene. 5-Hydroxymethylnorbornene. Cyclol



CAS Registry Number: 95-12-5

Molecular Formula: C₈H₁₂O

Molecular Weight: 124.182

Accurate Mass: 124.088815

Percentage Composition: C 77.38%; H 9.74%; O 12.88%

>>Variant: (1R,2R)-form

Synonym(s): (+)-endo-form

CAS Registry Number: 67671-06-1

Molecular Formula: C₈H₁₂O

Molecular Weight: 124.182

Accurate Mass: 124.088815

Percentage Composition: C 77.38%; H 9.74%; O 12.88%

Boiling Point: Bp_{11.2} 90-90.6°

Optical Rotation: [α]_D²⁵ +61.9 (c, 0.6 in 95% EtOH) (68% ee)

>>Variant: (1R,2S)-form

Synonym(s): (+)-exo-form

CAS Registry Number: 67671-05-0

Molecular Formula: C₈H₁₂O

Molecular Weight: 124.182

Accurate Mass: 124.088815

Percentage Composition: C 77.38%; H 9.74%; O 12.88%

Optical Rotation: [α]_D²⁵ +6 (c, 1.3 in 95% EtOH) (25% ee)

>>Variant: (1S,2R)-form

Synonym(s): (–)-exo-form

CAS Registry Number: 67505-46-8

Molecular Formula: C₈H₁₂O

Molecular Weight: 124.182

Accurate Mass: 124.088815

Percentage Composition: C 77.38%; H 9.74%; O 12.88%

Optical Rotation: [α]_D –23.9 (c, 1 in 95% EtOH)

>>Variant: (1S,2S)-form

Synonym(s): (–)-endo-form

CAS Registry Number: 42070-82-6

Molecular Formula: C₈H₁₂O

Molecular Weight: 124.182

Accurate Mass: 124.088815

Percentage Composition: C 77.38%; H 9.74%; O 12.88%

Boiling Point: Bp₁₁ 85-87°

Optical Rotation: [α]_D –95 (c, 1 in 95% EtOH)

>>Derivative: 4-Bromobenzenesulfonyl

Molecular Formula: C₁₄H₁₃BrO₃S

Molecular Weight: 343.241

Accurate Mass: 342.012526

Percentage Composition: C 48.99%; H 4.40%; Br 23.28%; O 13.98%; S 9.34%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 80.2-80.8°

Optical Rotation: [α]_D –13 (c, 4.1 in CHCl₃)