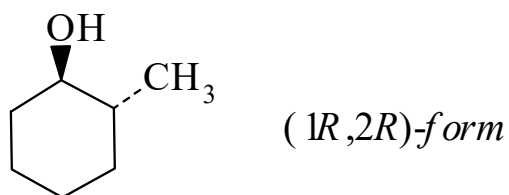




>>Entry Name: 2-Methylcyclohexanol, 9CI

Synonym(s): Hexahydro-*o*-cresol



CAS Registry Number: 583-59-5

Related CAS Registry Numbers(s): 7443-52-9 15963-35-6 25639-42-3

Extra CAS Registry Numbers(s): 25639-42-3

Molecular Formula: C₇H₁₄O

Molecular Weight: 114.187

Accurate Mass: 114.104465

Percentage Composition: C 73.63%; H 12.36%; O 14.01%

Hazard & Toxicity: Fl. p. 59/65°, autoignition temp. 296°. Mod. toxic by inhalation. Irritant

Aldrich: 24111-3

Fluka: 66320

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

Synonym(s): (–)-*trans*-form

CAS Registry Number: 19043-03-9

Molecular Formula: C₇H₁₄O

Molecular Weight: 114.187

Accurate Mass: 114.104465

Percentage Composition: C 73.63%; H 12.36%; O 14.01%

Boiling Point: Bp₂₉ 78-79°

Optical Rotation: [α]_D –39.5 (c, 0.43 in MeOH)

>>Derivative: Acid phthalate

Physical Description: Cryst. (AcOH or C₆H₆)

Melting Point: Mp 97-98°

Optical Rotation: [α]_D –38.7 (C₆H₆)

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

Synonym(s): (–)-*cis*-form

CAS Registry Number: 19043-02-8

Molecular Formula: C₇H₁₄O

Molecular Weight: 114.187

Accurate Mass: 114.104465

Percentage Composition: C 73.63%; H 12.36%; O 14.01%

Boiling Point: Bp₂₀ 78°

Optical Rotation: [α]_D –9.8 (c, 3.8 in CHCl₃)

>>Derivative: Acid phthalate

Physical Description: Cryst. (AcOH or C₆H₆)

Melting Point: Mp 122°

Optical Rotation: [α]_D –63.5 (C₆H₆). [α]_D –10.7 (CHCl₃)

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

Synonym(s): (+)-*cis*-form

CAS Registry Number: 15963-35-6

Molecular Formula: C₇H₁₄O

Molecular Weight: 114.187

Accurate Mass: 114.104465

Percentage Composition: C 73.63%; H 12.36%; O 14.01%

Melting Point: Mp 25-26.5°

Boiling Point: Bp₁₀ 59°

Optical Rotation: [α]_D +21.8 (neat)