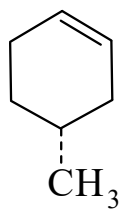




>>Entry Name: 4-Methylcyclohexene, 9CI



(*R*)-form

CAS Registry Number: 591-47-9

Extra CAS Registry Numbers(s): 1335-86-0

Molecular Formula: C₇H₁₂

Molecular Weight: 96.172

Accurate Mass: 96.0939

Percentage Composition: C 87.42%; H 12.58%

Hazard & Toxicity: Highly flammable, fl. p. −1°(oc)

Aldrich: M3900-8

Fluka: 66450

>>Variant: (*R*)-form

CAS Registry Number: 5710-02-1

Molecular Formula: C₇H₁₂

Molecular Weight: 96.172

Accurate Mass: 96.0939

Percentage Composition: C 87.42%; H 12.58%

Optical Rotation: $[\alpha]_{\text{D}}^{22} +75$ (c, 0.62 in MeOH) (70% op)

>>Variant: (*S*)-form

CAS Registry Number: 5681-54-9

Molecular Formula: C₇H₁₂

Molecular Weight: 96.172

Accurate Mass: 96.0939

Percentage Composition: C 87.42%; H 12.58%

Physical Description: Liq.

Boiling Point: Bp 92-94°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -128.7$ (c, 4.59 in CHCl₃) (99% ee)

>>Variant: (±)-form

CAS Registry Number: 26293-22-1

Molecular Formula: C₇H₁₂

Molecular Weight: 96.172

Accurate Mass: 96.0939

Percentage Composition: C 87.42%; H 12.58%

Melting Point: Mp −121.1°. Fp −115.5°

Boiling Point: Bp₇₃₆ 100.8-101.5°

Solubility: Insol. H₂O; sol. EtOH

Density: d²⁰ 0.799

Refractive Index: n_D²⁰ 1.4414

References:

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