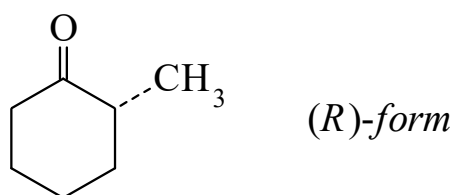




>>Entry Name: 2-Methylcyclohexanone, 9CI



CAS Registry Number: 583-60-8

Extra CAS Registry Numbers(s): 1331-22-2

Molecular Formula: C₇H₁₂O

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Hazard & Toxicity: Flammable, fl. p. 47°. LD₅₀ (rat, orl) 2140 mg/kg. LD₅₀ (rbt, skn) 1635 mg/kg. Eye and respiratory tract irritant. OES: long-term 50 ppm; short-term 75 ppm (sk)

Aldrich: M3840-0

Fluka: 66380

>>Variant: (R)-form

CAS Registry Number: 22554-29-6

Molecular Formula: C₇H₁₂O

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Optical Rotation: $[\alpha]_{\text{D}}^{20} -12.19$ (neat)

>>Variant: (S)-form

CAS Registry Number: 22554-27-4

Molecular Formula: C₇H₁₂O

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Boiling Point: Bp 166.5-168°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +12.3$ (MeOH). $[\alpha]_{\text{D}}^{25} +14.2$ (CHCl₃)

>>Variant: (±)-form

CAS Registry Number: 24965-84-2

Molecular Formula: C₇H₁₂O

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Physical Description: Oil

Melting Point: Fp -13.9°

Boiling Point: Bp 165-166°. Bp₂₀ 89-90°

Density: d_4^{20} 0.925

Refractive Index: n_{D}^{20} 1.4483

>>Derivative: Oxime

CAS Registry Number: 1122-26-5

Molecular Formula: C₇H₁₃NO

Molecular Weight: 127.186

Accurate Mass: 127.099714

Percentage Composition: C 66.11%; H 10.30%; N 11.01%; O 12.58%

Physical Description: Cryst.

Melting Point: Mp 43°

Boiling Point: Bp₁₃ 112-113°

>>Derivative: 2,4-Dinitrophenylhydrazone