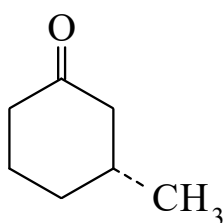




>>Entry Name: 3-Methylcyclohexanone, 9CI

Synonym(s): Hedeomol



(*R*)-form

CAS Registry Number: 591-24-2

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: Forms explosive peroxide with H₂O₂ + HNO₃. Eye and respiratory tract irritant

Aldrich: M3860-5

Fluka: 66390

>>Variant: (*R*)-form

CAS Registry Number: 13368-65-5

Molecular Formula: C₇H₁₂O

Molecular Weight: 112.171

Accurate Mass: 112.088815

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

Biological Source: Isol. from oil of *Hedeoma pulegioides* (pennyroyal), *Mentha* spp. and other oils

Boiling Point: Bp 169°. Bp₁₂ 68-70°

Aldrich: M3858-3

>>Derivative: Oxime

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 43-44°

Boiling Point: Bp 216-217°. Bp₁₈ 110°

>>Derivative: Semicarbazone

Physical Description: Plates (MeOH)

Melting Point: Mp 180°

Optical Rotation: $[\alpha]_{\text{D}}^{23} -27$ (EtOH)

>>Variant: (*S*)-form

CAS Registry Number: 24965-87-5

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 164-168°. Bp₁₅ 65°

>>Derivative: Semicarbazone

Melting Point: Mp 181°

Optical Rotation: $[\alpha]_{\text{D}}^{27} +30.5$

>>Variant: ($\pm$)-form