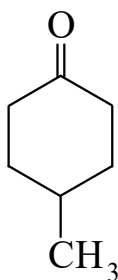




>>Entry Name: 4-Methylcyclohexanone, 9CI



CAS Registry Number: 589-92-4

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%

Biological Source: Present in various plant spp.

Melting Point: Fp -40.6°

Boiling Point: Bp 170°

Density: d₄²⁰ 0.914

Refractive Index: n_D²⁰ 1.4451

Hazard & Toxicity: Detonates with HNO₃ at 75°. LD₅₀ (rat, orl) 800 mg/kg. Eye and respiratory tract irritant

Aldrich: 17361-4

Fluka: 66400

>>Derivative: Oxime

CAS Registry Number: 4994-13-2

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 37-39°

Boiling Point: Bp₁₄ 114°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 5138-32-9

Physical Description: Orange cryst. (EtOH aq.)

Melting Point: Mp 133-134°

>>Derivative: Semicarbazone

CAS Registry Number: 5439-97-4

Physical Description: Prisms (MeOH)

Melting Point: Mp 197°

>>Derivative: Enol acetate

Synonym(s): 1-Acetoxy-4-methylcyclohexene

CAS Registry Number: 22422-17-9

Molecular Formula: C₉H₁₄O₂

Molecular Weight: 154.208

Accurate Mass: 154.09938

Percentage Composition: C 70.10%; H 9.15%; O 20.75%

Boiling Point: Bp₃₈ 99-100°. Bp₃ 53-56°

References: