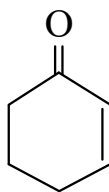




>>Entry Name: 2-Cyclohexen-1-one, 9CI



CAS Registry Number: 930-68-7

Extra CAS Registry Numbers(s): 25512-62-3

Molecular Formula: C₆H₈O

Molecular Weight: 96.129

Accurate Mass: 96.057515

Percentage Composition: C 74.97%; H 8.39%; O 16.64%

Source/Synthesis: Found in tobacco smoke condensate

Physical Description: Liq.

Boiling Point: Bp 169-171°. Bp₁₄ 61-63°

Refractive Index: n_D²⁷ 1.4838

Hazard & Toxicity: Eye irritant. LD₅₀ (rat, orl) 220 mg/kg. LD₅₀ (rbt, skn) 70 mg/kg

Aldrich: C10281-4

Fluka: 29255

>>Derivative: Oxime

Molecular Formula: C₆H₉NO

Molecular Weight: 111.143

Accurate Mass: 111.068414

Percentage Composition: C 64.84%; H 8.16%; N 12.60%; O 14.40%

Physical Description: Yellow needles

Melting Point: Mp 94-95°

Other Data: Mixt. of *E*, *Z*-isomers

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Orange needles (EtOH aq.)

Melting Point: Mp 168°

>>Derivative: Semicarbazone

Physical Description: Cryst. (MeOH)

Melting Point: Mp 171-172°

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