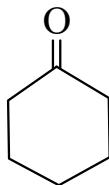




>>Entry Name: Cyclohexanone, 9CI

Synonym(s): Ketocyclohexane. Oxocyclohexane



CAS Registry Number: 108-94-1

Molecular Formula: C₆H₁₀O

Molecular Weight: 98.144

Accurate Mass: 98.073165

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

Source/Synthesis: Manuf. by oxidn. of Cyclohexanol [CXZ69-U](#)

Biological Source: Present in various plant spp.

Use/Importance: Solvent, swelling agent for PVC, synthetic intermediate. Used in the manuf. of Hexahydro-2*H*-azepin-2-one [DBR16-B](#) for nylon-6 and of Hexanedioic acid [DFV47-H](#) for nylon-66 prodn. Condensation polymers with formaldehyde are used in coating applications. H acceptor in Oppenauer oxidns. Used as a solvent in extraction-photometric detns. and in extraction separation of Ga, In, Hg, Bi

Physical Description: Oily liq.

Melting Point: Mp -45° (-32°)

Boiling Point: Bp 155°. Bp₁₅ 47°

Solubility: Mod. sol. H₂O

Density: d₄²⁰ 0.948

pKa Value: pK_a 16.7

Refractive Index: n_D²⁰ 1.4500

Hazard & Toxicity: Flammable, fl. p. 43°, autoignition temp. 420°. Forms explosive peroxide with H₂O₂. Eye, skin and respiratory tract irritant. Inhalation causes conjunctival irritation, and olfactory and respiratory system changes. LD₅₀ (rat, orl) 1535 mg/kg. Exp. reprod. effects. CNS depressant at high vapour conc. OES: long-term 25 ppm; short-term 100 ppm

Aldrich: 39824-1

Fluka: 29135

Sigma: C6301

Supelco: 44-2532

>>Derivative: Oxime

CAS Registry Number: 100-64-1

Molecular Formula: C₆H₁₁NO

Molecular Weight: 113.159

Accurate Mass: 113.084064

Percentage Composition: C 63.69%; H 9.80%; N 12.38%; O 14.14%

Physical Description: Prisms

Melting Point: Mp 89-90°

Boiling Point: Bp 206-210°

Solubility: Sol. H₂O, EtOH

Aldrich: C10220-2

Fluka: 29180

>>Derivative: *O*-Methyloxime

CAS Registry Number: 13858-85-0

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: Liq.

Boiling Point: Bp₂₀ 56-61°