



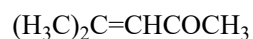
>>Entry Name: 4-Methyl-3-penten-2-one, 9CI

ENTRY UNDER REVIEW

Synonym(s): Isopropylideneacetone. Mesityl oxide. FEMA 3368

CAS Registry Number: 141-79-7

Related CAS Registry Numbers(s): 2158-24-9



Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}$

Molecular Weight: 98.144

Accurate Mass: 98.073165

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

Biological Source: Constit. of *Capsicum* spp., *Osmanthus fragrans* and other plants

Use/Importance: Solv. for nitrocellulose and vinyl resins. Intermed. for heterocyclic synth. Used as a solvent in extraction-separation of elements, e.g. Cr(VI), Ga, Ge, Mo, W, U, V, Zn, Cd, Pb (from HCl or KI/H₂SO₄ media). Flavouring ingredient

Physical Description: Liq. with odour of honey

Melting Point: Mp -41.5° (-59°)

Boiling Point: Bp $130-131^\circ$. Bp₃₇ 50°

Solubility: Spar. sol. H₂O

Density: d_4^{25} 0.851

pKa Value: $\text{p}K_a$ 0.25 (25° , 0.2M HClO₄)

Refractive Index: n_D^{13} 1.4484

Hazard & Toxicity: Flammable, fl. p. 31° , autoignition temp. 340° . Eye, skin and respiratory tract irritant. High vapour conc. narcotic. Contact with liq. can damage eyes. Prolonged or repeated exposure can injure liver, kidneys, and lungs, and cause dermatitis. LD₅₀ (rat, oral) 1120 mg/kg. OES: long-term 15 ppm; short-term 25 ppm

Aldrich: 28183-2

Fluka: 63940

Sigma: M2543

>>Derivative: E-Oxime

CAS Registry Number: 28052-09-7

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}$

Molecular Weight: 113.159

Accurate Mass: 113.084064

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

Boiling Point: Bp $184-187^\circ$. Bp₂ 70° . Bp₁₀ 85°

Other Data: Unstable isomer, sepd. with difficulty from the Z-form

>>Derivative: Z-Oxime

CAS Registry Number: 28052-10-0

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}$

Molecular Weight: 113.159

Accurate Mass: 113.084064

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

Physical Description: Cryst. (H₂O)

Melting Point: Mp 49°

Boiling Point: Bp₁₃ 102°

Other Data: Stable isomer

>>Derivative: 4-Nitrophenylhydrazone

CAS Registry Number: 88903-27-9

Physical Description: Orange needles (EtOH aq.)

Melting Point: Mp 207°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 964-83-0

Physical Description: Carmine cryst. (EtOH)

Melting Point: Mp 200°

References: