



>>Entry Name: Acetone

ENTRY UNDER REVIEW

Synonym(s): 2-Propanone, 9CI. Dimethyl ketone. FEMA 3326

CAS Registry Number: 67-64-1

Related CAS Registry Numbers(s): 666-52-4 43022-03-3

H_3CCOCH_3

Molecular Formula: $\text{C}_3\text{H}_6\text{O}$

Molecular Weight: 58.08

Accurate Mass: 58.041865

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Biological Source: A common constit. of plant tissues, e.g. *Ribes nigrum* volatiles. Produced industrially mainly by oxidation of Isopropylbenzene [HFN88-Y](#)

Use/Importance: Widely used solvent. Major industrial intermed. used in manuf. of other solvs., methacrylates and 2,2'-Bis(4-hydroxyphenyl)propane [DZN19-W](#). Forms acetonides with diols and Schiff bases with amines for gc or ms anal. Important industrial chemical, 41st in order of volume for USA in 1994 (production 1.39 million tons/year)

Physical Description: Volatile liq.

Melting Point: Mp -94°

Boiling Point: Bp 56.2°

Solubility: Misc. H_2O , org. solvs.

Density: d_{25}^{25} 0.79

Refractive Index: n_D^{20} 1.3588

Other Data: Crit. temp. 246.1°

Hazard & Toxicity: Highly flammable, fl. p. -19° , autoignition temp. 538° . Reacts vigorously with CHCl_3 in presence of base. Liquid is severe eye irritant and defats skin. High vapour conc. irritate respiratory tract. Inhalation of vapour initially causes excitement followed by CNS depression with headache, restlessness and fatigue. Coma may result. Exp. reprod. effects by inhalation. OES: long-term 750 ppm; short-term 1500 ppm

Aldrich: 32396-9

Fluka: 585

Sigma: A4206

Supelco: R80-1000

>>Derivative: Oxime

Synonym(s): Acetoxime

CAS Registry Number: 127-06-0

Molecular Formula: $\text{C}_3\text{H}_7\text{NO}$

Molecular Weight: 73.094

Accurate Mass: 73.052764

Percentage Composition: C 49.30%; H 9.65%; N 19.16%; O 21.89%

Use/Importance: Used for photometric detn. of Pt(II)

Physical Description: Cryst. (EtOH)

Melting Point: Mp 61°

Boiling Point: Bp $134-135^\circ$

Solubility: Sol. H_2O , EtOH , Et_2O , Me_2CO

pKa Value: pK_a 12.42 (25°)

Aldrich: A1050-7

Fluka: 750

Sigma: A2125

>>Derivative: O-(Benzyloxycarbonyl)oxime

CAS Registry Number: 137160-76-0

Molecular Formula: $\text{C}_{11}\text{H}_{13}\text{NO}_3$

Molecular Weight: 207.229

Accurate Mass: 207.089544

Percentage Composition: C 63.76%; H 6.32%; N 6.76%; O 23.16%

Physical Description: Cryst. (hexane)

Melting Point: Mp $46-48^\circ$

>>Derivative: Hydrazone

see 2-Propanone hydrazone, [LXZ26-A](#)