



>>Entry Name: 3-Methyl-2-butanone, 9CI

Synonym(s): Isopropyl methyl ketone. Isopentanone. 2-Acetylpropane

CAS Registry Number: 563-80-4

$(\text{H}_3\text{C})_2\text{CHCOCH}_3$

Molecular Formula: $\text{C}_5\text{H}_{10}\text{O}$

Molecular Weight: 86.133

Accurate Mass: 86.073165

Percentage Composition: C 69.72%; H 11.70%; O 18.58%

Biological Source: Isol. from various plant spp.

Boiling Point: Bp 93-94°

Density: d_4^{16} 0.805

Refractive Index: n_D^{16} 1.3879

Hazard & Toxicity: Skin and eye irritant. LD₅₀ (rat, orl) 148 mg/kg

Aldrich: 23861-9

Fluka: 59600

Rare Chemicals Library: S55737-4

>>Derivative: Oxime

CAS Registry Number: 600-20-4

Molecular Formula: $\text{C}_5\text{H}_{11}\text{NO}$

Molecular Weight: 101.148

Accurate Mass: 101.084064

Percentage Composition: C 59.37%; H 10.96%; N 13.85%; O 15.82%

Boiling Point: Bp 157-158°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 3077-97-2

Physical Description: Orange-yellow cryst.

Melting Point: Mp 117°

>>Derivative: Semicarbazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 114°

>>Derivative: Di-Et acetal

Synonym(s): 2,2-Diethoxy-3-methylbutane

Molecular Formula: $\text{C}_9\text{H}_{20}\text{O}_2$

Molecular Weight: 160.256

Accurate Mass: 160.14633

Percentage Composition: C 67.45%; H 12.58%; O 19.97%

Boiling Point: Bp₂₀ 52.4°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 632A, (nmr)

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