



>>Entry Name: **2-Hexanone**, 9CI

Synonym(s): Butyl methyl ketone. Methyl butyl ketone

CAS Registry Number: 591-78-6

$\text{H}_3\text{C}(\text{CH}_2)_3\text{COCH}_3$

Molecular Formula: $\text{C}_6\text{H}_{12}\text{O}$

Molecular Weight: 100.16

Accurate Mass: 100.088815

Percentage Composition: C 71.95%; H 12.08%; O 15.97%

Biological Source: Present in hop oil (*Humulus lupulus*), potato (*Solanum tuberosum*) and ground nuts (*Arachis hypogaea*)

Physical Description: Liq.

Boiling Point: Bp 127°

Density: d^0 0.83

Hazard & Toxicity: Flammable, fl. p. 23°, autoignition temp. 423°. Eye and skin irritant. Chronic exposure associated with development of peripheral neuropathies. Earlier symptoms of exp. include headache and nausea. LD₅₀ (rat, orl) 2590 mg/kg. OES: long-term 5 ppm (Sk)

Aldrich: 10300-4

Fluka: 20270

Supelco: R43-4110

>>Derivative: Oxime

CAS Registry Number: 5577-48-0

Molecular Formula: $\text{C}_6\text{H}_{13}\text{NO}$

Molecular Weight: 115.175

Accurate Mass: 115.099714

Percentage Composition: C 62.57%; H 11.38%; N 12.16%; O 13.89%

Boiling Point: Bp 185° (slight dec.). Bp₁₁₂ 138°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 2348-17-6

Melting Point: Mp 117-118° (106°)

>>Derivative: Semicarbazone

CAS Registry Number: 3622-64-8

Melting Point: Mp 125°

>>Derivative: Di-Et ketal

Synonym(s): 2,2-Diethoxyhexane

Molecular Formula: $\text{C}_{10}\text{H}_{22}\text{O}_2$

Molecular Weight: 174.283

Accurate Mass: 174.16198

Percentage Composition: C 68.92%; H 12.72%; O 18.36%

Boiling Point: Bp₁₈ 68-69°

References:

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