



>>Entry Name: 3-Hexanone, 9CI

ENTRY UNDER REVIEW

Synonym(s): Ethyl propyl ketone. FEMA 3290

CAS Registry Number: 589-38-8

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

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%

Use/Importance: Flavouring ingredient

Boiling Point: Bp 123-123.5°

Solubility: Sl. sol. H_2O , sd. Me_2CO , EtOH, Et_2O

Density: d^{20}_4 0.81

Refractive Index: n^{20}_D 1.4004

Hazard & Toxicity: Highly flammable, fl. p. 14°. Eye and skin irritant. LD₅₀ (rat, orl) 3360 mg/kg

Aldrich: 10302-0

Fluka: 4760

>>Derivative: Oxime

CAS Registry Number: 28364-56-9

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: Bp₁₇ 86°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 1655-39-6

Melting Point: Mp 130°. Mp 149-151°

>>Derivative: Semicarbazone

CAS Registry Number: 3622-65-9

Melting Point: Mp 112°

References:

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