



>>Entry Name: 3-Heptanone, 9CI

ENTRY UNDER REVIEW

Synonym(s): Butyl ethyl ketone. FEMA 2545

CAS Registry Number: 106-35-4

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

Molecular Formula: $\text{C}_7\text{H}_{14}\text{O}$

Molecular Weight: 114.187

Accurate Mass: 114.104465

Percentage Composition: C 73.63%; H 12.36%; O 14.01%

Use/Importance: Flavouring ingredient

Physical Description: Liq. with a powerful green, fatty, fruity odour and a melon, banana flavour

Boiling Point: Bp 149-152°

Density: d^{20}_4 0.82

Refractive Index: n^{20}_D 1.4115

Hazard & Toxicity: Flammable. Eye and skin irritant. LD₅₀ (rat, orl) 2760 mg/kg. OES: long-term 50 ppm; short-term 75 ppm (Sk) (current); short-term 100 ppm (Sk) (proposed)

Aldrich: H315-1

Fluka: 3220

Sigma: H6511

>>Derivative: Oxime

CAS Registry Number: 2108-81-8

Molecular Formula: $\text{C}_7\text{H}_{15}\text{NO}$

Molecular Weight: 129.202

Accurate Mass: 129.115364

Percentage Composition: C 65.07%; H 11.70%; N 10.84%; O 12.38%

Boiling Point: Bp₁ 56°

>>Derivative: Semicarbazone

CAS Registry Number: 3622-67-1

Melting Point: Mp 99-100°. Mp 111°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 64739-11-3

Melting Point: Mp 70.2°

References:

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