



>>Entry Name: 5-Methyl-2-hexanone, 9CI

ENTRY UNDER REVIEW

Synonym(s): Isoamyl methyl ketone

CAS Registry Number: 110-12-3

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

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%

Source/Synthesis: Volatile component in fruit pulp of papaya (*Carica papaya*), black tea aroma and in cooked beef and egg aroma

Boiling Point: Bp 144°

Density: d^{17} 0.818

Hazard & Toxicity: Flammable. Eye and skin irritant (slight). LD₅₀ (rat, orl) 4760 mg/kg. OES: long-term 50 ppm; short-term 75 ppm (current): short-term 100 ppm (Sk) (proposed)

Aldrich: 11025-6

Fluka: 59140

Sigma: M8524

>>Derivative: Oxime

CAS Registry Number: 624-44-2

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%

Physical Description: Oil

Boiling Point: Bp 195-196°

>>Derivative: Semicarbazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 142-143°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Orange cryst.

Melting Point: Mp 95°

References:

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Marshall, A. *et al.*, *J. Am. Soc. Mass Spectrom.*, 1991, **2**, 292, (ms)

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