



>>Entry Name: **2,4-Dimethyl-3-pentanone**, 9CI

Synonym(s): Diisopropyl ketone. Isopropyl ketone. Isobutyron

CAS Registry Number: 565-80-0

Type of Compound Code(s): VA1050

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

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%

Biological Source: Isol. from lavender oil (*Lavendula officinalis* hybrid)

Physical Description: Liq.

Boiling Point: Bp 124-125°

Density: d_4^{20} 0.811

Refractive Index: n_D^{20} 1.4001

Hazard & Toxicity: Highly flammable, fl. p. 15°. LD₅₀ (rat, orl) 3536 mg/kg

Aldrich: 13686-7

Fluka: 38430

>>Derivative: Oxime

CAS Registry Number: 1113-74-2

Type of Compound Code(s): PA3150 PM6860

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%

Use/Importance: Used for extraction-photometric detn. of Pd

Physical Description: Needles (EtOH)

Melting Point: Mp 34°

Boiling Point: Bp 181-185°. Bp₁₂ 82-85°

Solubility: Sol. alcohols

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 7153-35-7

Melting Point: Mp 94-98°

>>Derivative: Semicarbazone

CAS Registry Number: 5338-14-7

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 160°

References:

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