



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

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

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:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **1**, 634C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 407C, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 489C, (*ir*)

Aldrich Library of NMR Spectra, **2**, 106D, (*pmr*)

Pfeiffer, G.J. *et al.*, *J.A.C.S.*, 1931, **53**, 1043, (*props*)

Hauser, C.R. *et al.*, *J.A.C.S.*, 1937, **59**, 1823, (*synth*)

Stadler, P.A., *Helv. Chim. Acta*, 1960, **43**, 1601, (*isol*)

Dunn, P.J. *et al.*, *Mikrochim. Acta*, 1975, **2**, 129, (*oxime, detn, Pd*)

Cooks, R.G. *et al.*, *J.A.C.S.*, 1976, **98**, 2011, (*ms*)

Andrieu, C.G. *et al.*, *Org. Magn. Reson.*, 1978, **11**, 528, (*cmr*)

Boulton, A.J. *et al.*, *J.C.S. Perkin I*, 1987, 2073, (*oxime*)

Konaka, S. *et al.*, *J. Phys. Chem.*, 1990, **94**, 1793, (*ir, Raman, ed, conformn*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DTI600