



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

Synonym(s): Methyl neopentyl ketone

CAS Registry Number: 590-50-1

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

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%

Boiling Point: Bp 126.4°

Aldrich: 13687-5

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 4602-24-8

Physical Description: Cryst. (MeOH)

Melting Point: Mp 99.3-100°

References:

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

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

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

Casey, C.P. *et al.*, *Tet. Lett.*, 1973, 2071, (*synth*)

Seebach, D. *et al.*, *Annalen*, 1977, 830, (*synth*)

Carlson, R. *et al.*, *Acta Chem. Scand., Ser. B*, 1978, **32**, 85, (*synth*)

House, H.O. *et al.*, *J.O.C.*, 1978, **43**, 2443, (*synth*)