



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

CAS Registry Number: 5497-67-6

H2C=CHCH2C(CH3)2CHO

Molecular Formula: C₇H₁₂O

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Physical Description: Liq.

Boiling Point: Bp 124-126°

Aldrich: 29097-1

>>Derivative: Oxime

CAS Registry Number: 10533-71-8

Molecular Formula: C₇H₁₃NO

Molecular Weight: 127.186

Accurate Mass: 127.099714

Percentage Composition: C 66.11%; H 10.30%; N 11.01%; O 12.58%

Physical Description: Liq.

Boiling Point: Bp₂ 64-65°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Cryst.

Melting Point: Mp 117-118°

>>Derivative: Di-Me acetal

Synonym(s): 5,5-Dimethoxy-4,4-dimethyl-1-pentene

Molecular Formula: C₉H₁₈O₂

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Physical Description: Liq.

Boiling Point: Bp 164°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 736B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 560A, (*ir*)

Brannock, K.C., *J.A.C.S.*, 1959, **81**, 3379, (*synth*)

House, H.O. *et al.*, *J.O.C.*, 1974, **39**, 3102; 1976, **41**, 863, (*synth, ir, pmr, ms*)

Magnus, P. *et al.*, *Synth. Commun.*, 1980, **10**, 273, (*synth*)

Lewis, R.T. *et al.*, *Tetrahedron*, 1995, **51**, 3289, (*di-Me acetal*)