



>>Entry Name: 1-Phenyl-1-pentanone, 9CI

Synonym(s): Valerophenone, 8CI. *n*-Butyl phenyl ketone. 1-Benzoylbutane

CAS Registry Number: 1009-14-9

PhCOCH2CH2CH2CH3

Molecular Formula: C₁₁H₁₄O

Molecular Weight: 162.231

Accurate Mass: 162.104465

Percentage Composition: C 81.44%; H 8.70%; O 9.86%

Biological Source: Found in tobacco smoke, oakmoss and celery

Physical Description: Liq.

Boiling Point: Bp₂₅ 135-140°

Aldrich: V65-9

Fluka: 94595

Sigma: V8753

>>Derivative: Oxime

CAS Registry Number: 69060-55-5

Molecular Formula: C₁₁H₁₅NO

Molecular Weight: 177.246

Accurate Mass: 177.115364

Percentage Composition: C 74.54%; H 8.53%; N 7.90%; O 9.03%

Physical Description: Needles (EtOH aq. or petrol)

Melting Point: Mp 52-52.5°

Boiling Point: Bp₁₃ 163-165°

Solubility: Sol. EtOH, C₆H₆, spar. sol. petrol

>>Derivative: Semicarbazone

Synonym(s): 2-(1-Phenylpentylidene)hydrazinecarboxamide

Physical Description: Needles (EtOH)

Melting Point: Mp 166° (157-157.5°)

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Orange-red cryst. (EtOH)

Melting Point: Mp 123-124° (166°)

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 803B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 9C, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1229C, (*ir*)

Pfeiffer, P. *et al.*, *J. Prakt. Chem.*, 1924, **108**, 341, (*oxime*)

Shriner, R.L. *et al.*, *J.A.C.S.*, 1930, **52**, 1267, (*synth*)

Milstein, D. *et al.*, *J.A.C.S.*, 1978, **100**, 3636, (*synth*)

Yamashita, M. *et al.*, *Tet. Lett.*, 1978, 761, (*synth*)