



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

Synonym(s): Heptanophenone, 8CI. Hexyl phenyl ketone. Enanthophenone. Oenanthophenone. 1-Benzoylhexane

CAS Registry Number: 1671-75-6

$\text{PhCO}(\text{CH}_2)_5\text{CH}_3$

Molecular Formula:  $\text{C}_{13}\text{H}_{18}\text{O}$

Molecular Weight: 190.285

Accurate Mass: 190.135765

Percentage Composition: C 82.06%; H 9.53%; O 8.41%

Melting Point: Mp 17°

Boiling Point: Bp<sub>34</sub> 173°

Density:  $d_4^{20}$  0.9505

Aldrich: 15991-3

>>Derivative: Oxime

CAS Registry Number: 69060-57-7

Molecular Formula:  $\text{C}_{13}\text{H}_{19}\text{NO}$

Molecular Weight: 205.299

Accurate Mass: 205.146664

Percentage Composition: C 76.06%; H 9.33%; N 6.82%; O 7.79%

Physical Description: Needles (EtOH)

Melting Point: Mp 55°

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 137-139°

#### References:

*Aldrich Library of  $^{13}\text{C}$  and  $^1\text{H}$  FT NMR Spectra*, 1992, **2**, 804B, (*nmr*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 1230B, (*ir*)

*Aldrich Library of Infrared Spectra*, 3rd edn., 1981, 854F, (*ir*)

Krafft, F., *Ber.*, 1886, **19**, 2987, (*synth*)

Michnowicz, J. *et al.*, *Org. Mass Spectrom.*, 1972, **6**, 283, (*ms*)