



>>Entry Name: 2-Methyl-1-phenyl-1-propanone, 9CI

Synonym(s): Isobutyrophenone. Isopropyl phenyl ketone. Isobutyrylbenzene. 2-Benzoylpropane

CAS Registry Number: 611-70-1

PhCOCH(CH₃)₂

Molecular Formula: C₁₀H₁₂O

Molecular Weight: 148.204

Accurate Mass: 148.088815

Percentage Composition: C 81.04%; H 8.16%; O 10.80%

Physical Description: Liq.

Boiling Point: Bp₇₄₆ 220°. Bp₄ 86°

Aldrich: 13036-2

Fluka: 59730

>>Derivative: (E)-Oxime

CAS Registry Number: 72846-70-9

Molecular Formula: C₁₀H₁₃NO

Molecular Weight: 163.219

Accurate Mass: 163.099714

Percentage Composition: C 73.59%; H 8.03%; N 8.58%; O 9.80%

Physical Description: Prisms (pentane)

Melting Point: Mp 96°

>>Derivative: (Z)-Oxime

CAS Registry Number: 72846-71-0

Physical Description: Plates (pentane)

Melting Point: Mp 90°

>>Derivative: (E)-Phenylhydrazone

CAS Registry Number: 59130-84-6

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 29.5-30°

>>Derivative: Semicarbazone

Physical Description: Needles (EtOH)

Melting Point: Mp 181°

References:

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

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Favorski, M.A. *et al.*, *C. R. Hebd. Seances Acad. Sci.*, 1926, **182**, 221

Oumhoff, A.I., *Bull. Soc. Chim. Fr.*, 1928, **43**, 568

Hudson, B.E. *et al.*, *J.A.C.S.*, 1941, **63**, 3163

Kissman, H.M. *et al.*, *J.A.C.S.*, 1950, **72**, 5322