



>>Entry Name: 1-(4-Chlorophenyl)-2-propanone

Synonym(s): (4-Chlorophenyl)acetone

CAS Registry Number: 5586-88-9

Structure by analogy with 1-(2-Chlorophenyl)-2-propanone, [BCY84-O](#)

Molecular Formula: C₉H₉ClO

Molecular Weight: 168.622

Accurate Mass: 168.034192

Percentage Composition: C 64.11%; H 5.38%; Cl 21.02%; O 9.49%

Physical Description: Pale yellow liq., cryst. on standing

Melting Point: Mp 6-8°

Boiling Point: Bp₃ 98°

Density: d₂₀²⁰ 1.14

Refractive Index: n_D²⁰ 1.5360

Rare Chemicals Library: S62038-6

Other: Oakwood: 2534, PB: C17040

>>Derivative: Oxime

CAS Registry Number: 1454-65-5

Molecular Formula: C₉H₁₀ClNO

Molecular Weight: 183.637

Accurate Mass: 183.045091

Percentage Composition: C 58.87%; H 5.49%; Cl 19.31%; N 7.63%; O 8.71%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 55-57°

>>Derivative: 2,4-Dinitrophenylhydrazone

CAS Registry Number: 21899-82-1

Physical Description: Cryst. (MeOH)

Melting Point: Mp 125°

>>Derivative: Semicarbazone

CAS Registry Number: 16236-49-0

Physical Description: Flakes

Melting Point: Mp 188-189°

References:

Nelson, K.L. *et al.*, *J.A.C.S.*, 1964, **86**, 684, (*synth*)

Ferreira, A.B.B. *et al.*, *J.C.S. Perkin 2*, 1978, 995, (*pmr*)

Vogt, H.-H. *et al.*, *Chem. Ber.*, 1981, **114**, 2884, (*cmr*)

Langhals, H. *et al.*, *Chem. Ber.*, 1981, **114**, 3813, (*oxime*)

Kosugi, M. *et al.*, *Bull. Chem. Soc. Jpn.*, 1984, **57**, 242, (*synth*, *pmr*, *ir*, *ms*)

Abd-El-Aziz, A.S. *et al.*, *J. Organomet. Chem.*, 1988, **348**, 95, (*pmr*)

Ohwada, T. *et al.*, *Tet. Lett.*, 1990, **46**, 7539, (*synth*)