



>>Entry Name: 4-Methylbenzophenone, 8Cl

Synonym(s): (4-Methylphenyl)phenylmethanone, 9Cl. Phenyl *p*-tolyl ketone. 4-Benzoyltoluene

CAS Registry Number: 134-84-9

Molecular Formula: C₁₄H₁₂O

Molecular Weight: 196.248

Accurate Mass: 196.088815

Percentage Composition: C 85.68%; H 6.16%; O 8.15%

Use/Importance: Fixative in perfumery

Physical Description: Cryst. (petrol) in two forms

Melting Point: Mp 59-60° (stable form). Mp 55° (metastable form)

Boiling Point: Bp 326°

Hazard & Toxicity: LD₅₀ (mus, ipr) 250 mg/kg

Aldrich: M2995-9

>>Derivative: (*E*)-Oxime

CAS Registry Number: 2998-91-6

Molecular Formula: C₁₄H₁₃NO

Molecular Weight: 211.263

Accurate Mass: 211.099714

Percentage Composition: C 79.59%; H 6.20%; N 6.63%; O 7.57%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 153-154°

>>Derivative: (*Z*)-Oxime

CAS Registry Number: 2998-92-7

Physical Description: Needles (EtOH)

Melting Point: Mp 136-137.5°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 886A, (*nmr*)

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Davies, A.G. *et al.*, *J.C.S.*, 1954, 3474, (*synth*)

Hugel, N.M. *et al.*, *Aust. J. Chem.*, 1979, **32**, 1511, (*nmr*)

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