



>>Entry Name: 4'-Nitroacetophenone, 8Cl
Synonym(s): 1-(4-Nitrophenyl)ethanone, 9Cl

CAS Registry Number: 100-19-6

Molecular Formula: C₈H₇NO₃
Molecular Weight: 165.148
Accurate Mass: 165.042594
Percentage Composition: C 58.18%; H 4.27%; N 8.48%; O 29.06%
Physical Description: Yellow prisms
Melting Point: Mp 80-81°
Boiling Point: Bp 145-152°. Bp_{1.5} 138°
pKa Value: pK_a -7.94 (25°, H₂SO₄)

Aldrich: N960-8
Fluka: 72620

>>Derivative: Oxime

CAS Registry Number: 10342-64-0
Molecular Formula: C₈H₈N₂O₃
Molecular Weight: 180.163
Accurate Mass: 180.053493
Percentage Composition: C 53.33%; H 4.48%; N 15.55%; O 26.64%
Melting Point: Mp 174°

>>Derivative: Phenylhydrazone

Physical Description: Cryst. (EtOH)
Melting Point: Mp 132°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 50A, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1264A, (*ir*)
Aldrich Library of IR Spectra, 769G, (*ir*)
Ford-Moore, A.H. *et al.*, *J.C.S.*, 1946, 679
Kim, J.K.S. *et al.*, *Acta Cryst. B*, 1973, **29**, 1141, (*cryst struct*)
Penner, G.H. *et al.*, *Can. J. Chem.*, 1989, **67**, 525, (*cmr*)