



>>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*)