



>>Entry Name: 3'-Nitroacetophenone, 8Cl
Synonym(s): 1-(3-Nitrophenyl)ethanone, 9Cl

CAS Registry Number: 121-89-1

Molecular Formula: $C_8H_7NO_3$
Molecular Weight: 165.148
Accurate Mass: 165.042594
Percentage Composition: C 58.18%; H 4.27%; N 8.48%; O 29.06%
Physical Description: Needles (EtOH)
Melting Point: Mp 81°
Boiling Point: Bp 202°. Bp₁₈ 167°
pKa Value: pK_a -7.62 (25°, H₂SO₄)
Other Data: Steam-volatile
Hazard & Toxicity: Eye and skin irritant. LD₅₀ (rat, orl) 3250 mg/kg

Aldrich: N938-1

Fluka: 72610

>>Derivative: Oxime

CAS Registry Number: 7471-32-1
Molecular Formula: $C_8H_8N_2O_3$
Molecular Weight: 180.163
Accurate Mass: 180.053493
Percentage Composition: C 53.33%; H 4.48%; N 15.55%; O 26.64%
Physical Description: Needles (H₂O)
Melting Point: Mp 131-132°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Orange cryst.
Melting Point: Mp 232.5-233°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 49D, (ir)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 872A, (nmr)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1263D, (ir)
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Feeder, N. *et al.*, *Acta Cryst. C*, 1996, **52**, 1454-1456, (cryst struct)
Bolte, M. *et al.*, *Acta Cryst. C*, 1997, **53**, 474-476, (synth struct)
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