



>>Entry Name: 3'-Nitroacetophenone, 8Cl

Synonym(s): 1-(3-Nitrophenyl)ethanone, 9Cl

CAS Registry Number: 121-89-1

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: 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: C₈H₈N₂O₃

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*)

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