



>>Entry Name: Benzoylnitromethane

Synonym(s): 2-Nitro-1-phenylethanone, 9Cl. α -Nitroacetophenone. ω -Nitroacetophenone

CAS Registry Number: 614-21-1

PhCOCH₂NO₂

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%

Melting Point: Mp 106°

Solubility: Mod. sol. warm H₂O

Aldrich: 30808-0

>>Derivative: Oxime

CAS Registry Number: 21205-24-3

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 46°

>>Derivative: Phenylhydrazone

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 105-105.5°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 871B, (*nmr*)

Thiele, J., *Annalen*, 1902, **325**, 1, (*synth*)

Fujise, S. *et al.*, *Ber.*, 1935, **68**, 1275, (*synth*)

Bachman, G.B. *et al.*, *J.A.C.S.*, 1959, **81**, 4882, (*synth*)

Jung, M.E. *et al.*, *J.O.C.*, 1987, **52**, 4570, (*synth*, *pmr*)

Ashwell, M.A. *et al.*, *Synthesis*, 1988, 229, (*synth*)

Rathore, R. *et al.*, *J.O.C.*, 1996, **61**, 627, (*synth*, *ir*, *pmr*, *cmr*)