



>>Entry Name: 3-(4-Nitrophenyl)-3-oxopropanoic acid

Synonym(s): 4-Nitro- β -oxobenzenepropanoic acid, 9CI. 4-Nitrobenzoylacetic acid

CAS Registry Number: 29285-16-3

Molecular Formula: C₉H₇NO₅

Molecular Weight: 209.158

Accurate Mass: 209.032424

Percentage Composition: C 51.68%; H 3.37%; N 6.70%; O 38.25%

Physical Description: Needles (C₆H₆)

Melting Point: Mp 132°. Mp 135 dec.°

pKa Value: pK_a 3.24 (H₂O)

>>Derivative: Me ester

CAS Registry Number: 59156-55-7

Molecular Formula: C₁₀H₉NO₅

Molecular Weight: 223.185

Accurate Mass: 223.048074

Percentage Composition: C 53.82%; H 4.06%; N 6.28%; O 35.84%

Physical Description: Prisms

Melting Point: Mp 106-107°

>>Derivative: Et ester

CAS Registry Number: 838-57-3

Molecular Formula: C₁₁H₁₁NO₅

Molecular Weight: 237.212

Accurate Mass: 237.063724

Percentage Composition: C 55.70%; H 4.67%; N 5.90%; O 33.72%

Physical Description: Needles (EtOH), yellow plates

Melting Point: Mp 73°. Mp 76°

Other Data: Another form, Mp 90°, may also exist

Aldrich: E4120-6

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1238C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 290C, (*ir*)

Bülow, C. *et al.*, *Ber.*, 1902, **35**, 931

Hay, R.W. *et al.*, *Aust. J. Chem.*, 1970, **23**, 1407, (*ir*)

Straub, T.S. *et al.*, *J.A.C.S.*, 1972, **94**, 8881, (*synth*)