



>>Entry Name: 5-Oxo-5-phenylpentanoic acid

Synonym(s): δ -Oxobenzene-pentanoic acid, 9Cl. Butyrophenone- γ -carboxylic acid. 4-Benzoylbutanoic acid

CAS Registry Number: 1501-05-9

PhCOCH₂CH₂CH₂COOH

Molecular Formula: C₁₁H₁₂O₃

Molecular Weight: 192.214

Accurate Mass: 192.078645

Percentage Composition: C 68.74%; H 6.29%; O 24.97%

Melting Point: Mp 127°

Solubility: Mod. sol. H₂O

Aldrich: B1268-7

Fluka: 12926

>>Derivative: Oxime

Molecular Formula: C₁₁H₁₃NO₃

Molecular Weight: 207.229

Accurate Mass: 207.089544

Percentage Composition: C 63.76%; H 6.32%; N 6.76%; O 23.16%

Melting Point: Mp 110°

>>Derivative: Semicarbazone

Melting Point: Mp 214-215°

>>Derivative: Me ester

CAS Registry Number: 1501-04-8

Molecular Formula: C₁₂H₁₄O₃

Molecular Weight: 206.241

Accurate Mass: 206.094295

Percentage Composition: C 69.89%; H 6.84%; O 23.27%

Physical Description: Oil

Melting Point: Mp -2°

Boiling Point: Bp₈ 147-148°

>>Derivative: Me ester, 2,4-dinitrophenylhydrazone

Melting Point: Mp 149°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 999A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 148A, (*ir*)

Yoho, C.W. *et al.*, *J.A.C.S.*, 1952, **74**, 5597, (*synth*)

Le Guillanton, G., *Bull. Soc. Chim. Fr.*, 1969, **82**, 871, (*synth*)

Maurin, J.K. *et al.*, *Acta Cryst. C*, 1994, **50**, 78, (*cryst struct, oxime*)