



>>Entry Name: 3-Oxo-4-phenylbutanoic acid

Synonym(s): β -Oxobenzenebutanoic acid, 9CI. 4-Phenylacetoacetic acid

CAS Registry Number: 25832-09-1

PhCH₂COCH₂COOH

Molecular Formula: C₁₀H₁₀O₃

Molecular Weight: 178.187

Accurate Mass: 178.062995

Percentage Composition: C 67.41%; H 5.66%; O 26.94%

>>Derivative: Cu salt

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 176-178°

>>Derivative: Me ester

Molecular Formula: C₁₁H₁₂O₃

Molecular Weight: 192.214

Accurate Mass: 192.078645

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

Boiling Point: Bp₃ 125°

>>Derivative: Et ester

CAS Registry Number: 718-08-1

Molecular Formula: C₁₂H₁₄O₃

Molecular Weight: 206.241

Accurate Mass: 206.094295

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

Boiling Point: Bp_{0.03} 99-102°

Other Data: Said to exist as a mixt. of two enol forms

>>Derivative: 2,4-Dinitrophenylhydrazone

Melting Point: Mp 155°

>>Derivative: Semicarbazone

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 113-116°

>>Derivative: Anil

Molecular Formula: C₁₆H₁₅NO₂

Molecular Weight: 253.3

Accurate Mass: 253.110279

Percentage Composition: C 75.87%; H 5.97%; N 5.53%; O 12.63%

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 96-98.5°

References:

Sonn, A. *et al.*, *Ber.*, 1933, **66**, 1512, (*synth*)

Ames, G.R. *et al.*, *J.C.S.*, 1957, 3480, (*synth*)

Bram, G. *et al.*, *Bull. Soc. Chim. Fr.*, 1964, 945, (*synth*)

Angelo, B., *C. R. Hebd. Seances Acad. Sci.*, 1973, **276**, 293, (*synth*)

Numata, M. *et al.*, *J. Antibiot.*, 1978, **31**, 1245, (*synth*)