



>>Entry Name: 2-Oxo-4-phenylbutanoic acid

Synonym(s): α -Oxobenzenebutanoic acid, 9Cl. Benzylpyruvic acid

CAS Registry Number: 710-11-2

PhCH₂CH₂COCOOH

Molecular Formula: C₁₀H₁₀O₃

Molecular Weight: 178.187

Accurate Mass: 178.062995

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

Physical Description: Leaflets + 1½ H₂O (H₂O)

Melting Point: Mp 48-50° (sesquihydrate)

Solubility: Sol. hot H₂O

>>Derivative: Amide

Molecular Formula: C₁₀H₁₁NO₂

Molecular Weight: 177.202

Accurate Mass: 177.078979

Percentage Composition: C 67.78%; H 6.26%; N 7.90%; O 18.06%

Melting Point: Mp 180°

>>Derivative: Oxime

CAS Registry Number: 21486-56-6

Molecular Formula: C₁₀H₁₁NO₃

Molecular Weight: 193.202

Accurate Mass: 193.073894

Percentage Composition: C 62.17%; H 5.74%; N 7.25%; O 24.84%

Melting Point: Mp 165°

>>Derivative: Phenylhydrazone

Melting Point: Mp 144-145°

>>Derivative: Me ester

CAS Registry Number: 83402-87-3

Molecular Formula: C₁₁H₁₂O₃

Molecular Weight: 192.214

Accurate Mass: 192.078645

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

Boiling Point: Bp₂ 109-110°

>>Derivative: Et ester

CAS Registry Number: 64920-29-2

Molecular Formula: C₁₂H₁₄O₃

Molecular Weight: 206.241

Accurate Mass: 206.094295

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

Physical Description: Liq.

Boiling Point: Bp₂ 132°. Bp_{0.3} 105-110°

Refractive Index: n_D²⁰ 1.5050

References:

Moureu, H. *et al.*, *Bull. Soc. Chim. Fr.*, 1952, 442-445, (*synth*)

Cordier, P., *Bull. Soc. Chim. Fr.*, 1956, 564-569, (*synth*)

Anatol, J. *et al.*, *Synthesis*, 1971, **10**, 538-539, (*synth*)

Weinstock, L.M. *et al.*, *Synth. Commun.*, 1981, **11**, 943-946, (*Et ester*)

Blacklock, T.J. *et al.*, *J.O.C.*, 1988, **53**, 836-844, (*Et ester*)