



>>Entry Name: *N*-Benzoylglycine, 9CI

Synonym(s): Benzoylaminoacetic acid. Benzamidoacetic acid. Hippuric acid

CAS Registry Number: 495-69-2

Related CAS Registry Numbers(s): 532-94-5

PhCONHCH₂COOH

Molecular Formula: C₉H₉NO₃

Molecular Weight: 179.175

Accurate Mass: 179.058244

Percentage Composition: C 60.33%; H 5.06%; N 7.82%; O 26.79%

Biological Source: Naturally occurring amino acid found in the urine of most mammals including man. Urinary metab. of toluene, benzoic acid etc.

Use/Importance: Used in the azlactone synth. of aminoacids. Reference material used in elemental microanalysis

Physical Description: Needles (H₂O or EtOH), cryst. (CHCl₃/hexane)

Melting Point: Mp 187-188°

Solubility: Mod. sol. cold H₂O; sol. hot H₂O, EtOH; spar. sol. CHCl₃

pKa Value: pK_{a1} 3.59 (40°, 0.3M KCl)

Hazard & Toxicity: LD₅₀ (rat, ipr) 1500 mg/kg

Aldrich: 11200-3

Fluka: 53280

Sigma: H6375

>>Derivative: Me ester

CAS Registry Number: 1205-08-9

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%

Physical Description: Prisms

Melting Point: Mp 85°

Rare Chemicals Library: S75011-5

>>Derivative: Et ester

CAS Registry Number: 1499-53-2

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%

Physical Description: Needles (H₂O)

Melting Point: Mp 67.5°

Rare Chemicals Library: S67761-2

>>Derivative: Ph ester

CAS Registry Number: 2979-54-6

Molecular Formula: C₁₅H₁₃NO₃

Molecular Weight: 255.273

Accurate Mass: 255.089544

Percentage Composition: C 70.58%; H 5.13%; N 5.49%; O 18.80%

Physical Description: Plates (EtOH)

Melting Point: Mp 104°

>>Derivative: Benzyl ester

CAS Registry Number: 19811-58-6

Molecular Formula: C₁₆H₁₅NO₃

Molecular Weight: 269.299

Accurate Mass: 269.105194

Percentage Composition: C 71.36%; H 5.61%; N 5.20%; O 17.82%

Melting Point: Mp 87-89°