



>>Entry Name: *N*-Phenylglycine, 9Cl

Synonym(s): Anilinoacetic acid. (Phenylamino)acetic acid. Aniline-*N*-acetic acid

CAS Registry Number: 103-01-5

PhNHCH₂COOH

Molecular Formula: C₈H₉NO₂

Molecular Weight: 151.165

Accurate Mass: 151.063329

Percentage Composition: C 63.57%; H 6.00%; N 9.27%; O 21.17%

Use/Importance: Intermediate in the manuf. of Indigotin [BNC23-O](#)

Melting Point: Mp 127-128°

pKa Value: pK_{a1} 2; pK_{a2} 4.38 (25°,COOH)

Aldrich: 33046-9

Fluka: 78560

Rare Chemicals Library: S51916-2

Sigma: P7001

>>Derivative: Me ester

CAS Registry Number: 23284-84-6

Molecular Formula: C₉H₁₁NO₂

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Melting Point: Mp 48°

Rare Chemicals Library: S51480-2

>>Derivative: Et ester

CAS Registry Number: 2216-92-4

Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Melting Point: Mp 58°

Boiling Point: Bp 273-274°. Bp₈ 140°

>>Derivative: Ph ester

Molecular Formula: C₁₄H₁₃NO₂

Molecular Weight: 227.262

Accurate Mass: 227.094629

Percentage Composition: C 73.99%; H 5.77%; N 6.16%; O 14.08%

Physical Description: Leaflets (EtOH aq.)

Melting Point: Mp 82-83°

>>Derivative: Amide

Molecular Formula: C₈H₁₀N₂O

Molecular Weight: 150.18

Accurate Mass: 150.079313

Percentage Composition: C 63.98%; H 6.71%; N 18.65%; O 10.65%

Physical Description: Needles (H₂O), leaflets (EtOH)

Melting Point: Mp 136°

>>Derivative: Methylamide

Molecular Formula: C₉H₁₂N₂O

Molecular Weight: 164.207

Accurate Mass: 164.094963

Percentage Composition: C 65.83%; H 7.37%; N 17.06%; O 9.74%

Physical Description: Leaflets (EtOH aq.)

Melting Point: Mp 118°