



>>Entry Name: (Diphenylmethyleneimino)acetic acid

Synonym(s): *N*-(Diphenylmethylene)glycine, 9CI

CAS Registry Number: 136059-92-2

Related CAS Registry Numbers(s): 119244-11-0 119244-12-1 119244-13-2

Ph2C=NCH2COOH

Molecular Formula: C₁₅H₁₃NO₂

Molecular Weight: 239.273

Accurate Mass: 239.094629

Percentage Composition: C 75.30%; H 5.48%; N 5.85%; O 13.37%

Use/Importance: Used to prepare amino acids via phase-transfer alkylations

>>Derivative: Me ester

CAS Registry Number: 81167-39-7

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%

Melting Point: Mp 42.5-43°

>>Derivative: Et ester

CAS Registry Number: 69555-14-2

Molecular Formula: C₁₇H₁₇NO₂

Molecular Weight: 267.327

Accurate Mass: 267.125929

Percentage Composition: C 76.38%; H 6.41%; N 5.24%; O 11.97%

Use/Importance: Intermed. for the synth. of amino acids by selective mono- and dialkylation on the α -methylene

Melting Point: Mp 51-53°

pKa Value: p*K*_a 18.7 (DMSO)

Aldrich: 22254-2

Fluka: 43121

Sigma: D1519

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 81477-94-3

Molecular Formula: C₁₉H₂₁NO₂

Molecular Weight: 295.38

Accurate Mass: 295.157229

Percentage Composition: C 77.26%; H 7.17%; N 4.74%; O 10.83%

Melting Point: Mp 114-115° (111-112°)

Aldrich: 36448-7

>>Derivative: Benzyl ester

CAS Registry Number: 81477-91-0

Molecular Formula: C₂₂H₁₉NO₂

Molecular Weight: 329.398

Accurate Mass: 329.141579

Percentage Composition: C 80.22%; H 5.81%; N 4.25%; O 9.71%

Melting Point: Mp 91-92° (86.5-87°)

>>Derivative: Nitrile

Synonym(s): [(Diphenylmethylene)amino]acetonitrile, 9CI

CAS Registry Number: 70591-20-7

Molecular Formula: C₁₅H₁₂N₂

Molecular Weight: 220.273

Accurate Mass: 220.100048

Percentage Composition: C 81.79%; H 5.49%; N 12.72%

Melting Point: Mp 84-85° (81-82°)

Aldrich: 25265-4

Sigma: D7523

References: