



Extra CAS Registry Numbers(s): 2912-62-1 39478-47-2 40966-78-7
Molecular Formula: C₈H₈ClNO
Molecular Weight: 169.61
Accurate Mass: 169.029441
Percentage Composition: C 56.65%; H 4.75%; Cl 20.90%; N 8.26%; O 9.43%
Physical Description: Cryst. (as hydrochloride)
Melting Point: Mp 117 dec.° (hydrochloride)
Optical Rotation: $[\alpha]_D^{29} -116$ (c, 6 in 1M HCl)
Other Data: CAS no. refers to hydrochloride

>>Derivative: *N*-Ac

CAS Registry Number: 14257-84-2
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: Needles (H₂O)
Melting Point: Mp 191°
Optical Rotation: $[\alpha]_D^{20} +197.4$ (H₂O)

>>Derivative: *N*-*tert*-Butyloxycarbonyl

Synonym(s): α -[[[(1,1-Dimethylethoxy)carbonyl]amino]benzeneacetic acid, 9Cl

CAS Registry Number: 33125-05-2
Molecular Formula: C₁₃H₁₇NO₄
Molecular Weight: 251.282
Accurate Mass: 251.115759
Percentage Composition: C 62.14%; H 6.82%; N 5.57%; O 25.47%
Physical Description: Cryst. (hexane)
Melting Point: Mp 87-89.5°
Optical Rotation: $[\alpha]_D^{22} -148$ (c, 1 in EtOH)

>>Derivative: *N*-(3,5-Dinitrobenzoyl)

CAS Registry Number: 74927-72-3
Molecular Formula: C₁₅H₁₁N₃O₇
Molecular Weight: 345.268
Accurate Mass: 345.059702
Percentage Composition: C 52.18%; H 3.21%; N 12.17%; O 32.44%
Use/Importance: Used in chromatographic resoln. and assay of enantiomers
Melting Point: Mp 216-217°
Optical Rotation: $[\alpha]_D^{20} -102$ (c, 0.9 in THF)
Aldrich: 25003-1
Fluka: 42032
Sigma: D9270

>>Derivative: *N*-Benzyloxycarbonyl

Synonym(s): α -[[[(Phenylmethoxy)carbonyl]amino]benzeneacetic acid, 9Cl

CAS Registry Number: 17609-52-8
Molecular Formula: C₁₆H₁₅NO₄
Molecular Weight: 285.299
Accurate Mass: 285.100109
Percentage Composition: C 67.36%; H 5.30%; N 4.91%; O 22.43%
Physical Description: Cryst. (EtOH aq.)
Melting Point: Mp 130-135°
Optical Rotation: $[\alpha]_D^{21} -119$ (c, 4 in EtOH)

>>Derivative: *N*-Me

Synonym(s): 2-(Methylamino)-2-phenylacetic acid. α -(Methylamino)benzeneacetic acid, 9Cl. 2-Phenylsarcosine, 8Cl. *N*-Methyl-2-phenylglycine

CAS Registry Number: 30925-14-5
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%
Physical Description: Cryst. (Me₂CO aq.)
Melting Point: Mp 244 subl.°
Optical Rotation: $[\alpha]$