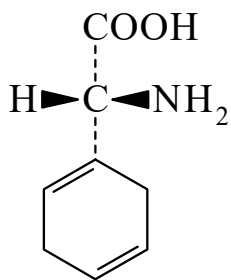




>>Entry Name: 2-Amino-2-(1,4-cyclohexadienyl)acetic acid

Synonym(s): α -Amino-1,4-cyclohexadiene-1-acetic acid, 9Cl. 2-(1,4-Cyclohexadienyl)glycine



Molecular Formula: C₈H₁₁NO₂

Molecular Weight: 153.18

Accurate Mass: 153.078979

Percentage Composition: C 62.73%; H 7.24%; N 9.14%; O 20.89%

>>Variant: (R)-form

Synonym(s): D-form

CAS Registry Number: 26774-88-9

Molecular Formula: C₈H₁₁NO₂

Molecular Weight: 153.18

Accurate Mass: 153.078979

Percentage Composition: C 62.73%; H 7.24%; N 9.14%; O 20.89%

Physical Description: Solid

Melting Point: Mp 296-297°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -117$ (c, 1 in 2M NaOH)

>>Derivative: Et ester

CAS Registry Number: 104236-46-6

Molecular Formula: C₁₀H₁₅NO₂

Molecular Weight: 181.234

Accurate Mass: 181.110279

Percentage Composition: C 66.27%; H 8.34%; N 7.73%; O 17.66%

Physical Description: Oil

Optical Rotation: $[\alpha]_{\text{D}}^{25} -3$ (c, 1 in CHCl₃)

>>Derivative: N-Ac

CAS Registry Number: 167424-24-0

Molecular Formula: C₁₀H₁₃NO₃

Molecular Weight: 195.218

Accurate Mass: 195.089544

Percentage Composition: C 61.53%; H 6.71%; N 7.17%; O 24.59%

Physical Description: Cryst. (EtOH/diisopropyl ether)

Optical Rotation: $[\alpha]_{\text{D}} -4$ (c, 1 in EtOH)

>>Derivative: N-Ac, Et ester

CAS Registry Number: 167424-25-1

Molecular Formula: C₁₂H₁₇NO₃

Molecular Weight: 223.271

Accurate Mass: 223.120844

Percentage Composition: C 64.55%; H 7.67%; N 6.27%; O 21.50%

Melting Point: Mp 80-81°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +78$ (c, 1 in CH₂Cl₂)

>>Derivative: N-Benzoyl

CAS Registry Number: 167424-31-9

Molecular Formula: C₁₅H₁₅NO₃

Molecular Weight: 257.288

Accurate Mass: 257.105194

Percentage Composition: C 70.02%; H 5.88%; N 5.44%; O 18.66%

Physical Description: Cryst.

Melting Point: Mp 173-174°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -14$ (c, 1 in 2M NaOH)