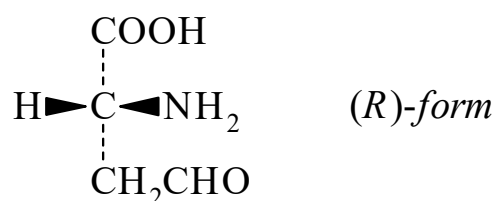




>>Entry Name: 2-Amino-4-oxobutanoic acid, 9CI

Synonym(s): 2-Aminosuccinaldehydic acid. Aspartyl semialdehyde. β -Formylalanine. Aspartic semialdehyde. β -Aspartaldehydic acid. Aspartal. ASA $\ddagger$. 2-Amino-4,4-dihydroxybutanoic acid



CAS Registry Number: 498-20-4

Molecular Formula: C₄H₇NO₃

Molecular Weight: 117.104

Accurate Mass: 117.042594

Percentage Composition: C 41.03%; H 6.02%; N 11.96%; O 40.99%

General Statement: Exists predominantly as the covalent hydrate in aq. soln. Fails to undergo normal aldehyde condensation reactions

>>Variant: (R)-form

Molecular Formula: C₄H₇NO₃

Molecular Weight: 117.104

Accurate Mass: 117.042594

Percentage Composition: C 41.03%; H 6.02%; N 11.96%; O 40.99%

>>Derivative: N-Benzyloxycarbonyl, Me ester

CAS Registry Number: 112229-40-0

Molecular Formula: C₁₃H₁₅NO₅

Molecular Weight: 265.265

Accurate Mass: 265.095024

Percentage Composition: C 58.86%; H 5.70%; N 5.28%; O 30.16%

Melting Point: Mp 161-163°

Optical Rotation: $[\alpha]_{\text{D}}$ -21 (in CHCl₃)

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 2338-03-6

Molecular Formula: C₄H₇NO₃

Molecular Weight: 117.104

Accurate Mass: 117.042594

Percentage Composition: C 41.03%; H 6.02%; N 11.96%; O 40.99%

Biological Source: Prod. by *Lyrus sativus*

Use/Importance: Biochemical intermed. in amino acid metab. Substrate for dihydropicolinate synthetase, an enzyme in the lysine biosynthetic pathway

Optical Rotation: $[\alpha]_{\text{D}}^{20}$ +3.2 (H₂O)

Other Data: Reasonably stable in acid soln., dec. in neutral soln. or on drying

>>Derivative: N-Benzyloxycarbonyl, Me ester

CAS Registry Number: 60684-59-5

Molecular Formula: C₁₃H₁₅NO₅

Molecular Weight: 265.265

Accurate Mass: 265.095024

Percentage Composition: C 58.86%; H 5.70%; N 5.28%; O 30.16%

Melting Point: Mp 161-163°

Optical Rotation: $[\alpha]_{\text{D}}$ +21 (in CHCl₃)

>>Derivative: N-Phthaloyl, Me ester

CAS Registry Number: 137278-36-5

Molecular Formula: C₁₃H₁₃NO₅

Molecular Weight: 263.249

Accurate Mass: 263.079374

Percentage Composition: C 59.31%; H 4.98%; N 5.32%; O 30.39%

Use/Importance: Protected form of parent compd.

Physical Description: Solid

Melting Point: Mp 64-68°

Optical Rotation: $[\alpha]$