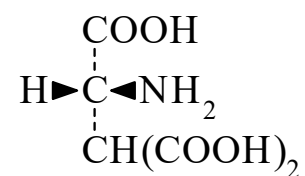




>>Entry Name: 2-Amino-1,1,2-ethanetricarboxylic acid, 9CI

Synonym(s): β -Carboxyaspartic acid. Asa $\ddagger$



(*R*)-form

CAS Registry Number: 75898-26-9

Related CAS Registry Numbers(s): 90365-27-8

Molecular Formula: C₅H₇NO₆

Molecular Weight: 177.113

Accurate Mass: 177.027339

Percentage Composition: C 33.91%; H 3.98%; N 7.91%; O 54.20%

General Statement: Obt. only in racemic form from natural systems

Sigma: C9272

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 99265-42-6

Molecular Formula: C₅H₇NO₆

Molecular Weight: 177.113

Accurate Mass: 177.027339

Percentage Composition: C 33.91%; H 3.98%; N 7.91%; O 54.20%

Source/Synthesis: Synthetic

>>Derivative: Hydrochloride

CAS Registry Number: 111934-05-5

Physical Description: Solid

Optical Rotation: $[\alpha]_{\text{D}}^{25} -13.25$ (c, 0.8 in H₂O)

>>Derivative: *N*-Ac, Tri-Me ester

CAS Registry Number: 99265-41-5

Molecular Formula: C₁₀H₁₅NO₇

Molecular Weight: 261.231

Accurate Mass: 261.084854

Percentage Composition: C 45.98%; H 5.79%; N 5.36%; O 42.87%

Optical Rotation: $[\alpha]_{\text{D}}^{20} +86.9$ (c, 2.0 in MeOH)

>>Derivative: 1,1-Di-*tert*-butyl ester, 2-Me ester

CAS Registry Number: 99166-13-9

Melting Point: Mp 63-64°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +0.4$ (c, 1.0 in MeOH)

>>Variant: ($\pm$)-form

CAS Registry Number: 78000-84-7

Molecular Formula: C₅H₇NO₆

Molecular Weight: 177.113

Accurate Mass: 177.027339

Percentage Composition: C 33.91%; H 3.98%; N 7.91%; O 54.20%

Biological Source: Isol. from the ribosomal proteins of *E. coli* and human atherosclerotic plaque

pKa Value: p*K*_a 1

Other Data: V. sensitive to decarboxylation so difficult to detect in natural systems

>>Derivative: Hydrochloride

CAS Registry Number: 78000-85-8

Other Data: Unstable