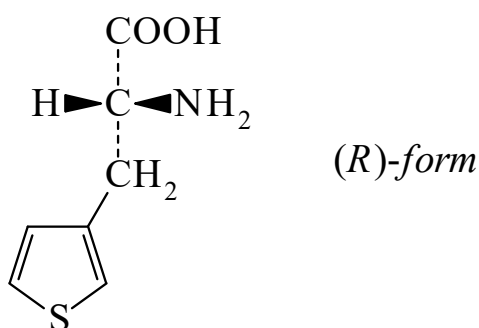




>>Entry Name: 2-Amino-3-(3-thienyl)propanoic acid

Synonym(s): α -Amino-3-thiophenepropanoic acid. β -3-Thienylalanine. 3-Thiophenealanine



CAS Registry Number: 22574-47-6

Molecular Formula: $C_7H_9NO_2S$

Molecular Weight: 171.22

Accurate Mass: 171.035399

Percentage Composition: C 49.10%; H 5.30%; N 8.18%; O 18.69%; S 18.73%

Use/Importance: Immunosuppressant in mice

>>Variant: (R)-form

CAS Registry Number: 152612-27-6

Molecular Formula: $C_7H_9NO_2S$

Molecular Weight: 171.22

Accurate Mass: 171.035399

Percentage Composition: C 49.10%; H 5.30%; N 8.18%; O 18.69%; S 18.73%

Physical Description: Solid (H_2O)

Melting Point: Mp 239-242°

Optical Rotation: $[\alpha]_D^{25} +42.6$ (c, 1 in H_2O) (>99% ee)

>>Derivative: Hydrochloride

CAS Registry Number: 152612-26-5

Physical Description: Solid (H_2O)

Melting Point: Mp 226-229°

Optical Rotation: $[\alpha]_D^{25} +23.2$ (c, 1 in H_2O) (99.6% ee)

>>Derivative: N-Ac

CAS Registry Number: 152612-25-4

Molecular Formula: $C_9H_{11}NO_3S$

Molecular Weight: 213.257

Accurate Mass: 213.045964

Percentage Composition: C 50.69%; H 5.20%; N 6.57%; O 22.51%; S 15.04%

Physical Description: Solid (H_2O)

Melting Point: Mp 176-178°

Optical Rotation: $[\alpha]_D^{25} -46.2$ (c, 1 in EtOH) (>99% ee)

>>Derivative: N-Benzoyl

CAS Registry Number: 89921-39-1

Molecular Formula: $C_{14}H_{13}NO_3S$

Molecular Weight: 275.328

Accurate Mass: 275.061614

Percentage Composition: C 61.07%; H 4.76%; N 5.09%; O 17.43%; S 11.65%

Melting Point: Mp 135°

Optical Rotation: $[\alpha]_D^{25} +4.1$ (c, 1 in EtOH) (96% ee)

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

CAS Registry Number: 3685-48-1

Molecular Formula: $C_7H_9NO_2S$

Molecular Weight: 171.22

Accurate Mass: 171.035399

Percentage Composition: C 49.10%; H 5.30%; N 8.18%; O 18.69%; S 18.73%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 265-267°