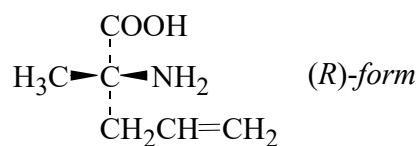




>>Entry Name: 2-Amino-2-methyl-4-pentenoic acid, 9CI

Synonym(s): α -Allylalanine



CAS Registry Number: 64298-91-5

Related CAS Registry Numbers(s): 142653-95-0

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}_2$

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

>>Variant: (R)-form

CAS Registry Number: 96886-56-5

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}_2$

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Physical Description: Cryst.

Melting Point: Mp 296-299°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +24.1$ (c, 0.7 in MeOH)

>>Variant: (S)-form

CAS Registry Number: 96886-55-4

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}_2$

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Melting Point: Mp 300 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -25.7$ (c, 0.8 in MeOH) (94% ee)

>>Derivative: Me ester

CAS Registry Number: 88820-87-5

Molecular Formula: $\text{C}_7\text{H}_{13}\text{NO}_2$

Molecular Weight: 143.185

Accurate Mass: 143.094629

Percentage Composition: C 58.72%; H 9.15%; N 9.78%; O 22.35%

Physical Description: Oil

Boiling Point: Bp₁₆ 100°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -1.5$ (c, 0.66 in EtOH)

>>Variant: (±)-form

CAS Registry Number: 109584-04-5

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}_2$

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Physical Description: Solid (as hydrochloride)

Melting Point: Mp 197 subl.° (hydrochloride)

References:

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Broxterman, Q.B. *et al.*, *J.O.C.*, 1992, **57**, 6286-6294, (*S*-form, *synth*)
Roos, E.C. *et al.*, *J.O.C.*, 1993, **58**, 3259, (*synth*, *pmr*, *cmr*)
Frauer, A. *et al.*, *J.O.C.*, 1994, **59**, 4215-4222, (*S*-form, *synth*, *pmr*)
Alonso, F. *et al.*, *J.C.S. Perkin I*, 1998, 257-268, (*R*-form, *synth*, *ir*, *pmr*, *cmr*)
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