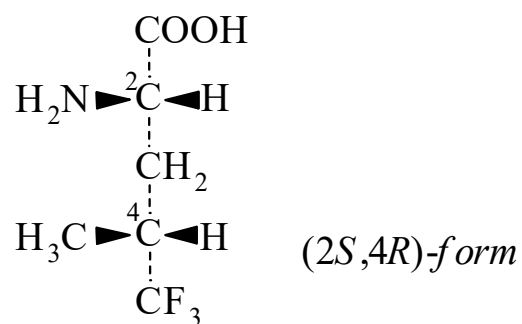




>>Entry Name: 2-Amino-5,5,5-trifluoro-4-methylpentanoic acid

Synonym(s): 5,5,5-Trifluoroleucine, 9Cl



CAS Registry Number: 372-22-5

Molecular Formula: C₆H₁₀F₃NO₂

Molecular Weight: 185.146

Accurate Mass: 185.066363

Percentage Composition: C 38.92%; H 5.44%; F 30.78%; N 7.57%; O 17.28%

Other: Oakwood 1540

>>Variant: (2*S*,4*R*)-form

CAS Registry Number: 96037-91-1

Molecular Formula: C₆H₁₀F₃NO₂

Molecular Weight: 185.146

Accurate Mass: 185.066363

Percentage Composition: C 38.92%; H 5.44%; F 30.78%; N 7.57%; O 17.28%

Physical Description: Microcryst. powder

Melting Point: Mp 243 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +17.6$ (c, 1 in H₂O)

>>Variant: (2*S*,4*S*)-form

CAS Registry Number: 96037-92-2

Molecular Formula: C₆H₁₀F₃NO₂

Molecular Weight: 185.146

Accurate Mass: 185.066363

Percentage Composition: C 38.92%; H 5.44%; F 30.78%; N 7.57%; O 17.28%

Melting Point: Mp 245 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -17$ (c, 1 in H₂O)

References:

Weinges, K. *et al.*, *Annalen*, 1985, 90, (*synth, pmr, cmr, cd*)

Taguchi, T. *et al.*, *Tet. Lett.*, 1986, 27, 5117, (*synth*)