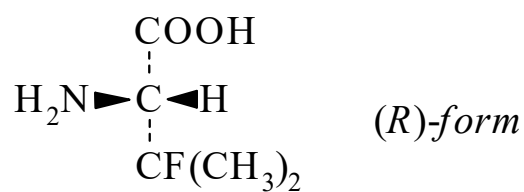




>>Entry Name: 2-Amino-3-fluoro-3-methylbutanoic acid

Synonym(s): 3-Fluorovaline, 9CI



CAS Registry Number: 43163-94-6

Molecular Formula: C₅H₁₀FNO₂

Molecular Weight: 135.138

Accurate Mass: 135.069557

Percentage Composition: C 44.44%; H 7.46%; F 14.06%; N 10.36%; O 23.68%

Fluka: 47581

>>Variant: (*R*)-form

Synonym(s): L-form

CAS Registry Number: 59752-74-8

Molecular Formula: C₅H₁₀FNO₂

Molecular Weight: 135.138

Accurate Mass: 135.069557

Percentage Composition: C 44.44%; H 7.46%; F 14.06%; N 10.36%; O 23.68%

Physical Description: Plates (2-Propanol aq.)

>>Variant: (±)-form

Molecular Formula: C₅H₁₀FNO₂

Molecular Weight: 135.138

Accurate Mass: 135.069557

Percentage Composition: C 44.44%; H 7.46%; F 14.06%; N 10.36%; O 23.68%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 204° (193-194°)

>>Derivative: Nitrile

CAS Registry Number: 79205-57-5

Molecular Formula: C₅H₉FN₂

Molecular Weight: 116.138

Accurate Mass: 116.074976

Percentage Composition: C 51.71%; H 7.81%; F 16.36%; N 24.12%

Physical Description: No phys. props. reported

References:

Gershon, H. *et al.*, *J. Med. Chem.*, 1973, **16**, 1407, (*synth*)

Kollonitsch, J. *et al.*, *J.O.C.*, 1976, **41**, 3107, (*synth*)

Ayi, A.I. *et al.*, *J. Fluorine Chem.*, 1984, **24**, 137, (*synth*)

Kaneko, C. *et al.*, *Chem. Pharm. Bull.*, 1995, **43**, 760, (*synth, pmr*)