



>>Entry Name: 3-Fluorophenylalanine, 9CI

Synonym(s): 2-Amino-3-(3-fluorophenyl)propanoic acid

CAS Registry Number: 456-88-2

Structure by analogy with 2-Fluorophenylalanine, [CJB83-K](#)

Molecular Formula: $C_9H_{10}FNO_2$

Molecular Weight: 183.182

Accurate Mass: 183.069557

Percentage Composition: C 59.01%; H 5.50%; F 10.37%; N 7.65%; O 17.47%

Hazard & Toxicity: LD₅₀ (mus, ipr) 5.9 mg/kg

>>Variant: (R)-form

Synonym(s): D-form

Molecular Formula: $C_9H_{10}FNO_2$

Molecular Weight: 183.182

Accurate Mass: 183.069557

Percentage Composition: C 59.01%; H 5.50%; F 10.37%; N 7.65%; O 17.47%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 230-234°

Optical Rotation: $[\alpha]_D^{25} +22$ (c, 2 in H₂O)

>>Derivative: N-Benzyloxycarbonyl

Melting Point: Mp 126-127°

Optical Rotation: $[\alpha]_D^{18} +7.35$ (c, 1 in MeOH)

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 19883-77-3

Molecular Formula: $C_9H_{10}FNO_2$

Molecular Weight: 183.182

Accurate Mass: 183.069557

Percentage Composition: C 59.01%; H 5.50%; F 10.37%; N 7.65%; O 17.47%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 239-243° (235-239°)

Optical Rotation: $[\alpha]_D^{18} -25.2$ (c, 1 in H₂O)

Fluka: 47306

>>Derivative: N-Benzyloxycarbonyl

Physical Description: Cryst. (diisopropyl ether)

Melting Point: Mp 124°

Optical Rotation: $[\alpha]_D^{20} -6.2$ (c, 1 in MeOH)

>>Variant: (±)-form

CAS Registry Number: 2629-54-1

Molecular Formula: $C_9H_{10}FNO_2$

Molecular Weight: 183.182

Accurate Mass: 183.069557

Percentage Composition: C 59.01%; H 5.50%; F 10.37%; N 7.65%; O 17.47%

Melting Point: Mp 240-250°. Mp 262-263°

Aldrich: 21943-6

Fluka: 47310

Sigma: F5126

>>Derivative: Hydrochloride

Melting Point: Mp 248-251 dec.°