



>>Entry Name: 3-Fluorotyrosine, 9CI

Synonym(s): 2-Amino-3-(3-fluoro-4-hydroxyphenyl)propanoic acid

CAS Registry Number: 139-26-4

Structure by analogy with 2-Fluorotyrosine, [BCR73-B](#)

Molecular Formula: C₉H₁₀FNO₃

Molecular Weight: 199.181

Accurate Mass: 199.064472

Percentage Composition: C 54.27%; H 5.06%; F 9.54%; N 7.03%; O 24.10%

Hazard & Toxicity: Human toxic effects at low oral doses

>>Variant: (S)-form

CAS Registry Number: 7423-96-3

Molecular Formula: C₉H₁₀FNO₃

Molecular Weight: 199.181

Accurate Mass: 199.064472

Percentage Composition: C 54.27%; H 5.06%; F 9.54%; N 7.03%; O 24.10%

Optical Rotation: $[\alpha]_{\text{D}}^{25} -7.72$ (c, 1 in 1M HCl)

Other Data: Used to label proteins for F-19 nmr studies

Fluka: 47574

>>Variant: (±)-form

CAS Registry Number: 403-90-7

Molecular Formula: C₉H₁₀FNO₃

Molecular Weight: 199.181

Accurate Mass: 199.064472

Percentage Composition: C 54.27%; H 5.06%; F 9.54%; N 7.03%; O 24.10%

Melting Point: Mp 278-280°

Aldrich: 13840-1

Sigma: F4505

>>Derivative: N-Benzoyl

Molecular Formula: C₁₆H₁₄FNO₄

Molecular Weight: 303.289

Accurate Mass: 303.090687

Percentage Composition: C 63.36%; H 4.65%; F 6.26%; N 4.62%; O 21.10%

Melting Point: Mp 221-222°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1189A, (*nmr*)

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Kraft, K., *Chem. Ber.*, 1951, **84**, 150, (*synth*)

Bashkir, E.A., *CA*, 1973, **78**, 30175p, (*synth*)

Kimber, B.J. *et al.*, *Biochemistry*, 1977, **16**, 3492, (*use*)

Nagasawa, T. *et al.*, *Eur. J. Biochem.*, 1981, **117**, 33, (*synth*)

Boschelli, F. *et al.*, *J. Biol. Chem.*, 1981, **256**, 11595, (*use*)

Chirakel, R. *et al.*, *J. Fluorine Chem.*, 1987, **37**, 267, (*synth*)

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