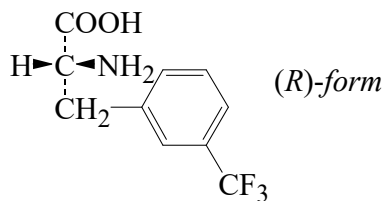




>>Entry Name: 2-Amino-3-(3-trifluoromethylphenyl)propanoic acid

Synonym(s): 3- Trifluoromethylphenylalanine, 9Cl. 3-(α,α,α -Trifluoro-*m*-tolyl)alanine, 8Cl



Related CAS Registry Numbers(s): 3832-75-5 3832-76-6 119349-14-3

Molecular Formula: C₁₀H₁₀F₃NO₂

Molecular Weight: 233.19

Accurate Mass: 233.066363

Percentage Composition: C 51.51%; H 4.32%; F 24.44%; N 6.01%; O 13.72%

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 14464-67-6

Molecular Formula: C₁₀H₁₀F₃NO₂

Molecular Weight: 233.19

Accurate Mass: 233.066363

Percentage Composition: C 51.51%; H 4.32%; F 24.44%; N 6.01%; O 13.72%

Melting Point: Mp 210-212°

Optical Rotation: $[\alpha]_{\text{D}}^{24} +14$ (c, 1 in H₂O)

>>Derivative: Hydrochloride

CAS Registry Number: 82317-79-1

Melting Point: Mp 208-210°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -19.7$ (c, 0.5 in MeOH)

>>Derivative: *N*-Ac, Me ester

CAS Registry Number: 82317-76-8

Molecular Formula: C₁₃H₁₄F₃NO₃

Molecular Weight: 289.254

Accurate Mass: 289.092578

Percentage Composition: C 53.98%; H 4.88%; F 19.70%; N 4.84%; O 16.59%

Melting Point: Mp 68-70°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -10$ (c, 1 in MeOH)

>>Derivative: *N*-*tert*-Butyloxycarbonyl

CAS Registry Number: 82317-82-6

Molecular Formula: C₁₅H₁₈F₃NO₄

Molecular Weight: 333.307

Accurate Mass: 333.118793

Percentage Composition: C 54.05%; H 5.44%; F 17.10%; N 4.20%; O 19.20%

Melting Point: Mp 100-102°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -7.1$ (c, 1 in MeOH)

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 14464-68-7

Molecular Formula: C₁₀H₁₀F₃NO₂

Molecular Weight: 233.19

Accurate Mass: 233.066363

Percentage Composition: C 51.51%; H 4.32%; F 24.44%; N 6.01%; O 13.72%

Melting Point: Mp 210-211°

Optical Rotation: $[\alpha]_{\text{D}}^{24} -14$ (c, 1 in H₂O)

>>Derivative: Hydrochloride

CAS Registry Number: 122839-48-9

Melting Point: Mp 230-232°