



>>Entry Name: 2-Amino-3-(4-trifluoromethylphenyl)acetic acid

Synonym(s): 4-Trifluoromethylphenylalanine, 9Cl. 3-(α,α,α ,-Trifluoro-*p*-tolyl)-alanine

Related CAS Registry Numbers(s): 114872-97-8 122839-56-9 123023-03-0 129941-39-5

Molecular Formula: $C_{10}H_{10}F_3NO_2$

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: 114872-99-0

Molecular Formula: $C_{10}H_{10}F_3NO_2$

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%

Optical Rotation: $[\alpha]_D^{22}$ -8.7 (c, 1 in MeOH)

>>Derivative: Hydrochloride (3:1)

CAS Registry Number: 82337-63-1

Melting Point: Mp 190-192°

Optical Rotation: $[\alpha]_D^{25}$ -1.7 (c, 0.5 in MeOH)

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

CAS Registry Number: 82317-77-9

Molecular Formula: $C_{13}H_{14}F_3NO_3$

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 98° (93-95°)

Optical Rotation: $[\alpha]_D^{22}$ -14.6 (c, 1 in EtOH)

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

CAS Registry Number: 82317-83-7

Molecular Formula: $C_{15}H_{18}F_3NO_4$

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 117-118°

Optical Rotation: $[\alpha]_D^{25}$ -4.8 (c, 1 in MeOH)

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 114926-38-4

Molecular Formula: $C_{10}H_{10}F_3NO_2$

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%

Optical Rotation: $[\alpha]_D^{22}$ +8.2 (c, 1 in MeOH)

>>Derivative: *N*-Ac

Melting Point: Mp 192°

Optical Rotation: $[\alpha]_D^{22}$ +4 (c, 1 in EtOH)