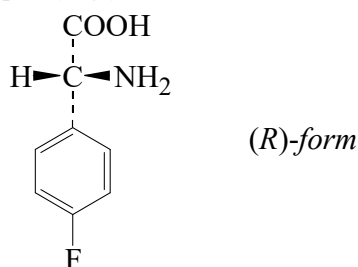




>>Entry Name: 2-Amino-2-(4-fluorophenyl)acetic acid

Synonym(s): α -Amino-4-fluorobenzeneacetic acid, 9Cl. 2-(*p*-Fluorophenyl)glycine



CAS Registry Number: 2343-28-4

Molecular Formula: C₈H₈FNO₂

Molecular Weight: 169.155

Accurate Mass: 169.053907

Percentage Composition: C 56.80%; H 4.77%; F 11.23%; N 8.28%; O 18.92%

>>Variant: (*R*)-form

CAS Registry Number: 93939-74-3

Molecular Formula: C₈H₈FNO₂

Molecular Weight: 169.155

Accurate Mass: 169.053907

Percentage Composition: C 56.80%; H 4.77%; F 11.23%; N 8.28%; O 18.92%

Optical Rotation: $[\alpha]_D^{22}$ -135 (c, 0.5 in 1M HCl)

>>Derivative: *N*-Ac

CAS Registry Number: 136814-99-8

Molecular Formula: C₁₀H₁₀FNO₃

Molecular Weight: 211.192

Accurate Mass: 211.064472

Percentage Composition: C 56.87%; H 4.77%; F 9.00%; N 6.63%; O 22.73%

Melting Point: Mp 180-181°

Optical Rotation: $[\alpha]_D^{20}$ -193.8 (c, 1 in MeOH) ($\geq$ 94% ee)

>>Variant: (*S*)-form

CAS Registry Number: 19883-57-9

Molecular Formula: C₈H₈FNO₂

Molecular Weight: 169.155

Accurate Mass: 169.053907

Percentage Composition: C 56.80%; H 4.77%; F 11.23%; N 8.28%; O 18.92%

Melting Point: Mp 295-300°

Optical Rotation: $[\alpha]_D^{20}$ +141 (c, 1 in 1M HCl) ($\geq$ 99.5% ee)

>>Variant: ($\pm$)-form

CAS Registry Number: 7292-73-1

Molecular Formula: C₈H₈FNO₂

Molecular Weight: 169.155

Accurate Mass: 169.053907

Percentage Composition: C 56.80%; H 4.77%; F 11.23%; N 8.28%; O 18.92%

Physical Description: Cryst.

Melting Point: Mp 271-273° (270-272°)

>>Derivative: *N*-Ac

CAS Registry Number: 153381-37-4

Extra CAS Registry Numbers(s): 68802-15-3

Molecular Formula: C₁₀H₁₀FNO₃

Molecular Weight: 211.192

Accurate Mass: 211.064472

Percentage Composition: C 56.87%; H 4.77%; F 9.00%; N 6.63%; O 22.73%

Physical Description: Cryst.

Melting Point: Mp 188-189.5°