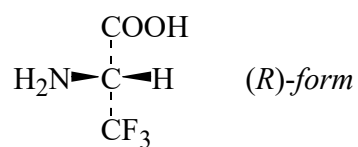




>> Name: 2-Amino-3,3,3-trifluoropropanoic acid

Synonym(s): 3,3,3-Trifluoroalanine, 9CI, 8CI



CAS Registry Number: 10065-69-7

Related CAS Registry Numbers(s): 127127-25-7 129939-36-2

Molecular Formula: $\text{C}_3\text{H}_4\text{F}_3\text{NO}_2$

Molecular Weight: 143.065

Accurate Mass: 143.019413

Percentage Composition: C 25.19%; H 2.82%; F 39.84%; N 9.79%; O 22.37%

>>Variant: (R)-form

CAS Registry Number: 129939-36-2

Molecular Formula: $\text{C}_3\text{H}_4\text{F}_3\text{NO}_2$

Molecular Weight: 143.065

Accurate Mass: 143.019413

Percentage Composition: C 25.19%; H 2.82%; F 39.84%; N 9.79%; O 22.37%

Physical Description: Cryst.

Optical Rotation: $[\alpha]_{\text{D}}^{23} +6.89$ (c, 0.76 in MeOH) (62% ee)

Other Data: Dec. $>210^\circ$

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

CAS Registry Number: 17463-43-3

Molecular Formula: $\text{C}_3\text{H}_4\text{F}_3\text{NO}_2$

Molecular Weight: 143.065

Accurate Mass: 143.019413

Percentage Composition: C 25.19%; H 2.82%; F 39.84%; N 9.79%; O 22.37%

Other Data: Subl. $>205^\circ$

Sigma: T5277

>>Derivative: Hydrochloride

CAS Registry Number: 96105-72-5

Melting Point: Mp 186 dec.°

>>Derivative: Me ester

CAS Registry Number: 27240-44-4

Molecular Formula: $\text{C}_4\text{H}_6\text{F}_3\text{NO}_2$

Molecular Weight: 157.092

Accurate Mass: 157.035063

Percentage Composition: C 30.58%; H 3.85%; F 36.28%; N 8.92%; O 20.37%

Physical Description: Oil

Boiling Point: Bp₁₂ $50\text{-}60^\circ$ (bath)

>>Derivative: Me ester, hydrochloride

CAS Registry Number: 134297-36-2

Melting Point: Mp 165°

>>Derivative: N-Benzoyl

CAS Registry Number: 1465-42-5

Molecular Formula: $\text{C}_{10}\text{H}_8\text{F}_3\text{NO}_3$

Molecular Weight: 247.173

Accurate Mass: 247.045628

Percentage Composition: C 48.59%; H 3.26%; F 23.06%; N 5.67%; O 19.42%

Physical Description: Cryst. (CHCl_3 /hexane/ Et_2O)

Melting Point: Mp $161\text{-}162^\circ$

References: