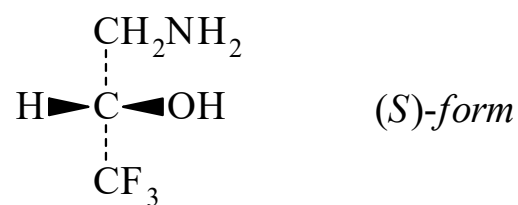




>>Entry Name: 3-Amino-1,1,1-trifluoro-2-propanol, 9CI

Synonym(s): 2-Hydroxy-3,3,3-trifluoropropylamine



CAS Registry Number: 431-38-9

Molecular Formula: C₃H₆F₃NO

Molecular Weight: 129.082

Accurate Mass: 129.040148

Percentage Composition: C 27.91%; H 4.68%; F 44.15%; N 10.85%; O 12.39%

>>Variant: (S)-form

CAS Registry Number: 160706-71-8

Molecular Formula: C₃H₆F₃NO

Molecular Weight: 129.082

Accurate Mass: 129.040148

Percentage Composition: C 27.91%; H 4.68%; F 44.15%; N 10.85%; O 12.39%

Physical Description: Solid

Melting Point: Mp 120-121°

Optical Rotation: $[\alpha]_{\text{D}}^{23} -19.54$ (c, 1.3 in MeOH) ($\geq 99\%$ ee)

>>Derivative: N,N-Di-Et

CAS Registry Number: 160595-63-1

Molecular Formula: C₇H₁₄F₃NO

Molecular Weight: 185.189

Accurate Mass: 185.102748

Percentage Composition: C 45.40%; H 7.62%; F 30.78%; N 7.56%; O 8.64%

Physical Description: Liq.

Boiling Point: Bp₄₀ 100° (Kugelrohr)

Optical Rotation: $[\alpha]_{\text{D}}^{22} -29.79$ (c, 1.4 in MeOH) (96% ee)

>>Variant: (±)-form

Molecular Formula: C₃H₆F₃NO

Molecular Weight: 129.082

Accurate Mass: 129.040148

Percentage Composition: C 27.91%; H 4.68%; F 44.15%; N 10.85%; O 12.39%

>>Derivative: Hydrochloride

Physical Description: Cryst.

Melting Point: Mp 147-148°

References:

Jones, R.G., *J.A.C.S.*, 1948, **70**, 143, (*synth*)

Ramachandran, P.V. *et al.*, *J.O.C.*, 1995, **60**, 41, (*synth, ir, pmr, cmr, F-19 nmr*)