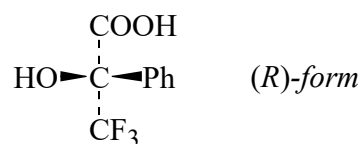




>>Entry Name: 3,3,3-Trifluoro-2-hydroxy-2-phenylpropanoic acid

Synonym(s): α -Hydroxy- α -(trifluoromethyl)benzeneacetic acid, 9CI. α -(Trifluoromethyl)mandelic acid, 8CI. β,β,β -Trifluoro- α -hydroxyhydratropic acid, 8CI. α -Hydroxy α -trifluoromethylphenylacetic acid



CAS Registry Number: 55519-22-7

Related CAS Registry Numbers(s): 20698-90-2 81655-41-6

Molecular Formula: $\text{C}_9\text{H}_7\text{F}_3\text{O}_3$

Molecular Weight: 220.148

Accurate Mass: 220.034729

Percentage Composition: C 49.10%; H 3.20%; F 25.89%; O 21.80%

>>Variant: (R)-form

CAS Registry Number: 17257-70-4

Molecular Formula: $\text{C}_9\text{H}_7\text{F}_3\text{O}_3$

Molecular Weight: 220.148

Accurate Mass: 220.034729

Percentage Composition: C 49.10%; H 3.20%; F 25.89%; O 21.80%

Optical Rotation: $[\alpha]_{\text{D}}^{20} -23.2$ (c, 2.93 in CHCl_3)

Other Data: +ve rotn. in MeOH or H_2O

>>Derivative: Me ether

Synonym(s): α -Methoxy- α -(trifluoromethyl)benzeneacetic acid, 9CI. β,β,β -Trifluoro- α -methoxyhydratropic acid, 8CI. Mosher's reagent. MTPA

CAS Registry Number: 20445-31-2

Molecular Formula: $\text{C}_{10}\text{H}_9\text{F}_3\text{O}_3$

Molecular Weight: 234.174

Accurate Mass: 234.050379

Percentage Composition: C 51.29%; H 3.87%; F 24.34%; O 20.50%

Use/Importance: Chiral nmr shift reagent and resolving agent. Reagent for determining optical purity of alcohols and amines

Boiling Point: $\text{Bp}_{1.5}$ 116-118°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +68.5$ (c, 1.49 in MeOH)

Aldrich: 15526-8

Fluka: 65362

Sigma: M9510

>>Derivative: Me ether, chloride

CAS Registry Number: 39637-99-5

Extra CAS Registry Numbers(s): 20445-33-4

Molecular Formula: $\text{C}_{10}\text{H}_8\text{ClF}_3\text{O}_2$

Molecular Weight: 252.62

Accurate Mass: 252.016491

Percentage Composition: C 47.55%; H 3.19%; Cl 14.03%; F 22.56%; O 12.67%

Use/Importance: Resolving agent for alcohols and amines

Boiling Point: Bp_1 54-56°

Optical Rotation: $[\alpha]_{\text{D}}^{24} +129$ (c, 5.7 in CCl_4)

Aldrich: 36967-5

Fluka: 65365

>>Variant: (S)-form

CAS Registry Number: 29246-94-4

Molecular Formula: $\text{C}_9\text{H}_7\text{F}_3\text{O}_3$

Molecular Weight: 220.148

Accurate Mass: 220.034729

Percentage Composition: C 49.10%; H 3.20%; F 25.89%; O 21.80%