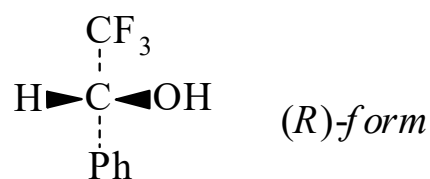




>>Entry Name: 2,2,2-Trifluoro-1-phenylethanol

Synonym(s): α -(Trifluoromethyl)benzenemethanol, 9CI. Phenyltrifluoromethylcarbinol



CAS Registry Number: 340-04-5

Molecular Formula: $\text{C}_8\text{H}_7\text{F}_3\text{O}$

Molecular Weight: 176.138

Accurate Mass: 176.044899

Percentage Composition: C 54.55%; H 4.01%; F 32.36%; O 9.08%

Use/Importance: Chiral solvating agent

Aldrich: 31986-4

>>Variant: (*R*)-form

CAS Registry Number: 10531-50-7

Molecular Formula: $\text{C}_8\text{H}_7\text{F}_3\text{O}$

Molecular Weight: 176.138

Accurate Mass: 176.044899

Percentage Composition: C 54.55%; H 4.01%; F 32.36%; O 9.08%

Melting Point: Mp 25°

Boiling Point: Bp_{0.6} 100-110°

Optical Rotation: $[\alpha]_{\text{D}}^{20}$ -40.5 (neat)

Aldrich: 41113-2

Fluka: 79231

>>Variant: (*S*)-form

CAS Registry Number: 340-06-7

Molecular Formula: $\text{C}_8\text{H}_7\text{F}_3\text{O}$

Molecular Weight: 176.138

Accurate Mass: 176.044899

Percentage Composition: C 54.55%; H 4.01%; F 32.36%; O 9.08%

Melting Point: Mp 25°

Boiling Point: Bp_{0.6} 100-110°

Optical Rotation: $[\alpha]_{\text{D}}^{23}$ +99 (c, 2.1 in CHCl_3) (92% ee). $[\alpha]_{\text{D}}^{20}$ +41.3 (neat)

Aldrich: 41114-0

Fluka: 79233

>>Derivative: Ac

Molecular Formula: $\text{C}_{10}\text{H}_9\text{F}_3\text{O}_2$

Molecular Weight: 218.175

Accurate Mass: 218.055464

Percentage Composition: C 55.05%; H 4.16%; F 26.12%; O 14.67%

Boiling Point: Bp_{0.7} 40-44°

Optical Rotation: $[\alpha]_{\text{D}}^{26}$ +96 (neat)

>>Derivative: Benzoyl

Molecular Formula: $\text{C}_{15}\text{H}_{11}\text{F}_3\text{O}_2$

Molecular Weight: 280.246

Accurate Mass: 280.071114

Percentage Composition: C 64.29%; H 3.96%; F 20.34%; O 11.42%

Boiling Point: Bp_{0.7} 110-114°

Optical Rotation: $[\alpha]_{\text{D}}^{24}$ -23 (neat)