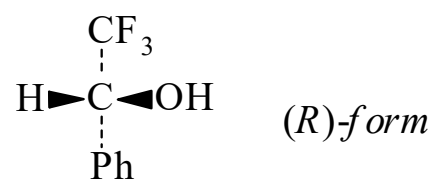




>>Entry Name: 2,2,2-Trifluoro-1-phenylethanol

Synonym(s):  $\alpha$ -(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<sub>0.6</sub> 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<sub>0.6</sub> 100-110°

Optical Rotation:  $[\alpha]_{\text{D}}^{23} +99$  (c, 2.1 in  $\text{CHCl}_3$ ) (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<sub>0.7</sub> 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<sub>0.7</sub> 110-114°

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