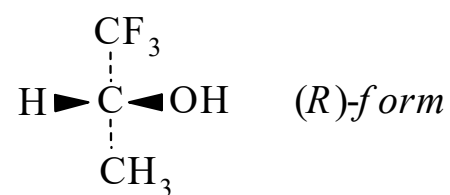




>>Entry Name: **1,1,1-Trifluoro-2-propanol**, 9CI, 8CI

Synonym(s): 1-(Trifluoromethyl)ethanol



CAS Registry Number: 374-01-6

Molecular Formula: C₃H₅F₃O

Molecular Weight: 114.067

Accurate Mass: 114.029249

Percentage Composition: C 31.59%; H 4.42%; F 49.97%; O 14.03%

Rare Chemicals Library: S43971-1

>>Variant: (R)-form

CAS Registry Number: 17628-73-8

Molecular Formula: C₃H₅F₃O

Molecular Weight: 114.067

Accurate Mass: 114.029249

Percentage Composition: C 31.59%; H 4.42%; F 49.97%; O 14.03%

Boiling Point: Bp₇₂₆ 75.8°

Optical Rotation: [α]_D²⁵ +2.17 (neat)

>>Variant: (S)-form

CAS Registry Number: 3539-97-7

Molecular Formula: C₃H₅F₃O

Molecular Weight: 114.067

Accurate Mass: 114.029249

Percentage Composition: C 31.59%; H 4.42%; F 49.97%; O 14.03%

Boiling Point: Bp₇₅₂ 77.7°

Optical Rotation: [α]_D²⁵ -5.65

>>Variant: (±)-form

CAS Registry Number: 17556-48-8

Molecular Formula: C₃H₅F₃O

Molecular Weight: 114.067

Accurate Mass: 114.029249

Percentage Composition: C 31.59%; H 4.42%; F 49.97%; O 14.03%

Physical Description: Liq.

Refractive Index: n_D²⁵ 1.3130

References:

Crawford, J.W.C., *J.C.S.*, 1965, 4280, (*synth, pmr, ir*)

Peters, H.M. *et al.*, *J.O.C.*, 1968, **33**, 4245, (*abs config*)

Crawford, J.W.C., *J.C.S.(C)*, 1969, 2332, (*synth*)

Drabicky, M.J. *et al.*, *J.O.C.*, 1976, 1472, (*synth*)

Ramachandran, P.V. *et al.*, *J.O.C.*, 1995, **60**, 41, (*synth*)