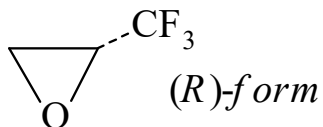




>>Entry Name: (Trifluoromethyl)oxirane, 9CI

Synonym(s): 1,1,1-Trifluoro-2,3-epoxypropane, 8CI. 2,3-Epoxy-1,1,1-trifluoropropane



CAS Registry Number: 359-41-1

Molecular Formula: $C_3H_3F_3O$

Molecular Weight: 112.051

Accurate Mass: 112.013599

Percentage Composition: C 32.16%; H 2.70%; F 50.87%; O 14.28%

>>Variant: (R)-form

Molecular Formula: $C_3H_3F_3O$

Molecular Weight: 112.051

Accurate Mass: 112.013599

Percentage Composition: C 32.16%; H 2.70%; F 50.87%; O 14.28%

Optical Rotation: $[\alpha]_D^{15} +11.9$ (c, 7.18 in $CHCl_3$)

>>Variant: (S)-form

CAS Registry Number: 130025-34-2

Molecular Formula: $C_3H_3F_3O$

Molecular Weight: 112.051

Accurate Mass: 112.013599

Percentage Composition: C 32.16%; H 2.70%; F 50.87%; O 14.28%

Boiling Point: Bp 39° approx.

Optical Rotation: $[\alpha]_D^{15} -12$ (c, 1.5 in $CHCl_3$)

>>Variant: (±)-form

Molecular Formula: $C_3H_3F_3O$

Molecular Weight: 112.051

Accurate Mass: 112.013599

Percentage Composition: C 32.16%; H 2.70%; F 50.87%; O 14.28%

Physical Description: Liq.

Boiling Point: Bp_{748.299988} 39.1-39.3°

Density: d_{20}^{20} 1.307

Refractive Index: n_D^{20} 1.2997

References:

McBee, E.T. *et al.*, *J.A.C.S.*, 1952, **74**, 3902, (*synth*)

Politzer, P. *et al.*, *Carcinogenesis (London)*, 1984, **5**, 845; *CA*, **101**, 105531, (*tox*)

von dem Bussche-Hünnefeld, C. *et al.*, *Chem. Ber.*, 1992, **125**, 2795

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