



>>Entry Name: 2,2,2-Trifluoroethanesulfonic acid, 9CI

CAS Registry Number: 1827-97-0

$\text{F}_3\text{CCH}_2\text{SO}_3\text{H}$

Molecular Formula: $\text{C}_2\text{H}_3\text{F}_3\text{O}_3\text{S}$

Molecular Weight: 164.105

Accurate Mass: 163.975499

Percentage Composition: C 14.64%; H 1.84%; F 34.73%; O 29.25%; S 19.54%

Melting Point: Mp 50-52°

Boiling Point: Bp_{0.5} 100°

Other Data: Hygroscopic

>>Derivative: Chloride

Synonym(s): 2,2,2-Trifluoroethanesulfonyl chloride. Tresyl chloride

CAS Registry Number: 1648-99-3

Molecular Formula: $\text{C}_2\text{H}_2\text{ClF}_3\text{O}_2\text{S}$

Molecular Weight: 182.551

Accurate Mass: 181.941611

Percentage Composition: C 13.16%; H 1.10%; Cl 19.42%; F 31.22%; O 17.53%; S 17.57%

Boiling Point: Bp₄₅ 65°

Aldrich: 32478-7

Fluka: 91691

Sigma: T6529

>>Derivative: Fluoride

Synonym(s): 2,2,2-Trifluoroethanesulfonyl fluoride. Tresyl fluoride

Molecular Formula: $\text{C}_2\text{H}_2\text{F}_4\text{O}_2\text{S}$

Molecular Weight: 166.096

Accurate Mass: 165.971162

Percentage Composition: C 14.46%; H 1.21%; F 45.75%; O 19.27%; S 19.31%

Boiling Point: Bp 100-101°

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1449B, (*nmr*)

U.S. Pat., 1961, 3 006 964; *CA*, **56**, 9967e, (*synth*)

Eleev, A.F. *et al.*, *CA*, 1979, **90**, 71701y, (*synth*)

Bunyagidj, C. *et al.*, *J.O.C.*, 1981, **46**, 3335

Smart, B.E. *et al.*, *J.A.C.S.*, 1987, **109**, 4982, (*fluoride*)