



>>Entry Name: Trifluoroethanethioic acid, 9Cl

Synonym(s): Trifluorothioacetic acid, 8Cl. Trifluorothiolacetic acid

CAS Registry Number: 2925-25-9

F₃CCOSH

Molecular Formula: C₂HF₃OS

Molecular Weight: 130.091

Accurate Mass: 129.970019

Percentage Composition: C 18.47%; H 0.77%; F 43.81%; O 12.30%; S 24.65%

Physical Description: Liq.

Boiling Point: Bp 35.5°

pKa Value: pK_a 0.78

>>Derivative: S-Me ester

Synonym(s): S-Methyl trifluorothioacetate

CAS Registry Number: 41879-94-1

Molecular Formula: C₃H₃F₃OS

Molecular Weight: 144.117

Accurate Mass: 143.985669

Percentage Composition: C 25.00%; H 2.10%; F 39.55%; O 11.10%; S 22.25%

Boiling Point: Bp 62-64°. Bp 71-72°

>>Derivative: S-Et ester

Synonym(s): S-Ethyl trifluorothioacetate

CAS Registry Number: 383-64-2

Molecular Formula: C₄H₅F₃OS

Molecular Weight: 158.144

Accurate Mass: 158.001319

Percentage Composition: C 30.38%; H 3.19%; F 36.04%; O 10.12%; S 20.28%

Use/Importance: Trifluoroacetylating agent

Boiling Point: Bp 90.5°

Aldrich: 17747-4

Fluka: 91876

Sigma: E4380

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1011A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 653D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 704D, (*ir*)

Sheppard, W.A. *et al.*, *J.O.C.*, 1960, **25**, 180, (*synth*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1972, **3**, 143

Bock, E. *et al.*, *Can. J. Chem.*, 1974, **52**, 3113, (*deriv*)