



>>Entry Name: 2,2,2-Trifluoroethanethiol, 9CI

Synonym(s): 1,1,1-Trifluoro-2-mercaptoethane

CAS Registry Number: 1544-53-2

$\text{F}_3\text{CCH}_2\text{SH}$

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

Molecular Weight: 116.107

Accurate Mass: 115.990754

Percentage Composition: C 20.69%; H 2.60%; F 49.09%; S 27.62%

Boiling Point: Bp 36.5°

Density: d 1.3

Refractive Index: n_D^{20} 1.3513

Aldrich: 37400-8

>>Derivative: S-Me

Synonym(s): 1,1,1-Trifluoro-2-(methylthio)ethane. Methyl 2,2,2-trifluoroethyl sulfide

CAS Registry Number: 5187-55-3

Molecular Formula: $\text{C}_3\text{H}_5\text{F}_3\text{S}$

Molecular Weight: 130.134

Accurate Mass: 130.006404

Percentage Composition: C 27.69%; H 3.87%; F 43.80%; S 24.64%

Boiling Point: Bp 67°

Refractive Index: n_D^{20} 1.3658

>>Derivative: S-Et

Synonym(s): 2-(Ethylthio)-1,1,1-trifluoroethane. Ethyl 2,2,2-trifluoroethyl sulfide

CAS Registry Number: 5187-62-2

Molecular Formula: $\text{C}_4\text{H}_7\text{F}_3\text{S}$

Molecular Weight: 144.161

Accurate Mass: 144.022054

Percentage Composition: C 33.33%; H 4.89%; F 39.54%; S 22.24%

Boiling Point: Bp 90°

Refractive Index: n_D^{20} 1.3778

>>Derivative: S-tert-Butyl

Synonym(s): *tert*-Butyl 2,2,2-trifluoroethyl sulfide. 2-(*tert*-Butylthio)-1,1,1-trifluoroethane

CAS Registry Number: 77745-01-8

Molecular Formula: $\text{C}_6\text{H}_{11}\text{F}_3\text{S}$

Molecular Weight: 172.214

Accurate Mass: 172.053354

Percentage Composition: C 41.85%; H 6.44%; F 33.10%; S 18.62%

Boiling Point: Bp₁₀₀ 70-72°

>>Derivative: S-Benzyl

Synonym(s): 2-(Benzylthio)-1,1,1-trifluoroethane. [[(2,2,2-Trifluoroethyl)thio]methyl]benzene. Benzyl 2,2,2-trifluoroethyl sulfide

CAS Registry Number: 77745-03-0

Molecular Formula: $\text{C}_9\text{H}_9\text{F}_3\text{S}$

Molecular Weight: 206.231

Accurate Mass: 206.037704

Percentage Composition: C 52.42%; H 4.40%; F 27.64%; S 15.55%

Boiling Point: Bp₂₀ 45-46°

Aldrich: 39633-8

Fluka: 13957

Sigma: B4917