



>>Entry Name: Ethanethioic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Thioacetic acid. Thiolacetic acid‡

CAS Registry Number: 507-09-5

$\text{H}_3\text{CCOSH} \leftrightarrow \text{H}_3\text{CC(S)OH}$

Molecular Formula: $\text{C}_2\text{H}_4\text{OS}$

Molecular Weight: 76.119

Accurate Mass: 75.998285

Percentage Composition: C 31.56%; H 5.30%; O 21.02%; S 42.13%

General Statement: Tautomeric. Forms 2 series of esters

Use/Importance: Radical addition reagent for alkenes and alkynes, *S*-acetylating agent

Physical Description: Liq. with pungent odour

Melting Point: Mp -17°

Boiling Point: Bp 93°

Solubility: Sol. H_2O , EtOH, Et_2O

Density: d^{20}_4 1.068

pKa Value: $\text{p}K_{\text{a}}$ 3.33 (25°)

Refractive Index: n^{20}_{D} 1.4630

Hazard & Toxicity: LD₅₀ (mus, ipr) 75 mg/kg. Flammable, fl. p. $<23^\circ$

Aldrich: T3080-5

Fluka: 88620

Sigma: T5375

>>Variant: *SH*-form

Molecular Formula: $\text{C}_2\text{H}_4\text{OS}$

Molecular Weight: 76.119

Accurate Mass: 75.998285

Percentage Composition: C 31.56%; H 5.30%; O 21.02%; S 42.13%

>>Derivative: Me ester

Synonym(s): *S*-Methyl thioacetate

CAS Registry Number: 1534-08-3

Molecular Formula: $\text{C}_3\text{H}_6\text{OS}$

Molecular Weight: 90.146

Accurate Mass: 90.013935

Percentage Composition: C 39.97%; H 6.71%; O 17.75%; S 35.57%

Boiling Point: Bp $95-96^\circ$

>>Derivative: Et ester

Synonym(s): *S*-Ethyl thioacetate. FEMA 3282

CAS Registry Number: 625-60-5

Molecular Formula: $\text{C}_4\text{H}_8\text{OS}$

Molecular Weight: 104.173

Accurate Mass: 104.029585

Percentage Composition: C 46.12%; H 7.74%; O 15.36%; S 30.78%

Use/Importance: Flavouring ingredient

Boiling Point: Bp $116-117^\circ$

Solubility: Insol., H_2O ; v. sol. EtOH, Et_2O

Density: d^{20}_4 0.98

Refractive Index: n^{21}_{D} 1.4583

Aldrich: W32820-0