



>>Entry Name: 2,2'-Thiobisacetic acid, 9CI

Synonym(s): 2,2'-Thiodiacetic acid, 8CI. Dimethyl sulfide dicarboxylic acid. Dicarboxydimethyl sulfide. Bis(carboxymethyl) sulfide. Thiodiglycollic acid

CAS Registry Number: 123-93-3

Related CAS Registry Numbers(s): 33388-14-6

HOOCCH₂SCH₂COOH

Molecular Formula: C₄H₆O₄S

Molecular Weight: 150.155

Accurate Mass: 149.99868

Percentage Composition: C 32.00%; H 4.03%; O 42.62%; S 21.36%

Physical Description: Cryst. (EtOAc/C₆H₆)

Melting Point: Mp 129°

Solubility: V. sol. H₂O; sol. EtOH

pKa Value: pK_a 3.32 (25°, H₂O)

Other Data: Polyamides and polyhydrazides contg. this acid have been synth.

Hazard & Toxicity: LD₅₀ (mus, ipr) 300 mg/kg

Aldrich: T3000-7

Fluka: 88570

Sigma: T6250

>>Derivative: Methiodide

Melting Point: Mp 189°

>>Derivative: Ethiodide

Melting Point: Mp 134°

>>Derivative: Di-Me ester

CAS Registry Number: 16002-29-2

Molecular Formula: C₆H₁₀O₄S

Molecular Weight: 178.209

Accurate Mass: 178.02998

Percentage Composition: C 40.44%; H 5.66%; O 35.91%; S 17.99%

Boiling Point: Bp₁₁ 135°

>>Derivative: Di-Et ester

CAS Registry Number: 925-47-3

Molecular Formula: C₈H₁₄O₄S

Molecular Weight: 206.262

Accurate Mass: 206.06128

Percentage Composition: C 46.59%; H 6.84%; O 31.03%; S 15.55%

Boiling Point: Bp 267-268°

Rare Chemicals Library: S59480-6

>>Derivative: Dichloride

Synonym(s): 2,2'-Thiobisacetyl chloride, 9CI

CAS Registry Number: 7646-91-5

Molecular Formula: C₄H₄Cl₂O₂S

Molecular Weight: 187.046

Accurate Mass: 185.930904

Percentage Composition: C 25.69%; H 2.16%; Cl 37.91%; O 17.11%; S 17.14%

Physical Description: Liq.

Other Data: Monomer for sulfur contg. polyamides