



>>Entry Name: 3,3'-Thiobispropanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3,3'-Thiodipropionic acid, 8CI. Thiodihydracrylic acid. Diethyl sulfide β,β' -dicarboxylic acid. Bis(2-carboxyethyl)sulfide. 4-Thiaheptanedioic acid

CAS Registry Number: 111-17-1

HOOCCH2CH2SCH2CH2COOH

Molecular Formula: $C_6H_{10}O_4S$

Molecular Weight: 178.209

Accurate Mass: 178.02998

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

Use/Importance: Antioxidant used in food packaging materials. Polyesters with diols are used as antioxidants for polymers

Melting Point: Mp 134°. Mp 129-130°

Solubility: Sol. H_2O , EtOH

pKa Value: pK_{a1} 3.84; pK_{a2} 4.66 (25°, 0.1M NaClO₄) pK_{a1} 4.15; pK_{a2} 4.8 (25°)

Hazard & Toxicity: Skin and eye irritant. LD₅₀ (rat, orl) 3980 mg/kg

Aldrich: T3020-1

Fluka: 88600

Sigma: T5264

>>Derivative: Di-Me ester

CAS Registry Number: 4131-74-2

Molecular Formula: $C_8H_{14}O_4S$

Molecular Weight: 206.262

Accurate Mass: 206.06128

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

Physical Description: Oil

Melting Point: Mp 7.8°

Boiling Point: Bp₁₀ 158-159°

Aldrich: D18830-1

>>Derivative: Di-Et ester

CAS Registry Number: 673-79-0

Molecular Formula: $C_{10}H_{18}O_4S$

Molecular Weight: 234.316

Accurate Mass: 234.09258

Percentage Composition: C 51.26%; H 7.74%; O 27.31%; S 13.68%

Physical Description: Oil

Melting Point: Mp -20°

Boiling Point: Bp₇ 148°

Rare Chemicals Library: S45940-2

>>Derivative: Dibutyl ester

CAS Registry Number: 6975-31-1

Molecular Formula: $C_{14}H_{26}O_4S$

Molecular Weight: 290.423

Accurate Mass: 290.15518

Percentage Composition: C 57.90%; H 9.02%; O 22.04%; S 11.04%

Physical Description: Oil

Boiling Point: Bp₂ 131°