



>>Entry Name: **3,3'-Thiobispropanol**, 9CI

Synonym(s): 3,3'-Thiodipropanol. Bis(3-hydroxypropyl) sulfide. 3,3-Dihydroxydipropyl sulfide. 4-Thia-1,7-heptanediol

CAS Registry Number: 10595-09-2

Related CAS Registry Numbers(s): 101810-61-1 102608-56-0 122560-18-3

HOCH₂CH₂CH₂SCH₂CH₂CH₂OH

Molecular Formula: C₆H₁₄O₂S

Molecular Weight: 150.241

Accurate Mass: 150.07145

Percentage Composition: C 47.97%; H 9.39%; O 21.30%; S 21.34%

Physical Description: Liq.

Boiling Point: Bp₁ 134-138°. Bp_{0.5} 140-142°

Density: d 1.09

Refractive Index: n_D²⁰ 1.5100

Aldrich: 20534-6

>>Derivative: Bis(phenylurethane)

Physical Description: Needles (C₆H₆)

Melting Point: Mp 122-123°

>>Derivative: Di-Ac

Molecular Formula: C₁₀H₁₈O₄S

Molecular Weight: 234.316

Accurate Mass: 234.09258

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

Boiling Point: Bp_{0.6} 129-134°

>>Derivative: Di-Ac, S,S-dioxide

Molecular Formula: C₁₀H₁₈O₆S

Molecular Weight: 266.315

Accurate Mass: 266.08241

Percentage Composition: C 45.10%; H 6.81%; O 36.05%; S 12.04%

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 53-55°

>>Derivative: Bis(methanesulfonyl)

CAS Registry Number: 75395-99-2

Molecular Formula: C₈H₁₈O₆S

Molecular Weight: 242.293

Accurate Mass: 242.08241

Percentage Composition: C 39.66%; H 7.49%; O 39.62%; S 13.23%

Physical Description: Cryst. (CH₂Cl₂/pentane)

Melting Point: Mp 42-43.5°

>>Derivative: Bis(4-methylbenzenesulfonyl)

CAS Registry Number: 101810-60-0

Molecular Formula: C₂₀H₂₆O₆S₃

Molecular Weight: 458.62

Accurate Mass: 458.08915

Percentage Composition: C 52.38%; H 5.71%; O 20.93%; S 20.98%

Physical Description: Cryst.

Melting Point: Mp 64-66°

References:

McGinnis, N.A. *et al.*, *J.C.S.*, 1941, 406, (*synth, di-Ac derivs*)

Searles, S. *et al.*, *J.A.C.S.*, 1951, **73**, 4515, (*synth*)

Kyba, E.P. *et al.*, *J.A.C.S.*, 1980, **102**, 7012-7014, (*synth, bismethanesulfonyl*)

Lange, S.J. *et al.*, *Tetrahedron*, 1995, **51**, 8175-8188, (*bis-4-methylbenzenesulfonyl*)

Loeb, S.J. *et al.*, *Can. J. Chem.*, 1996, **74**, 1377-1390, (*synth, pmr, cmr*)