



>>Entry Name: Di-*tert*-butyl disulfide

Synonym(s): Bis(1,1-dimethylethyl) disulfide, 9CI. *tert*-Butyl disulfide

CAS Registry Number: 110-06-5

Related CAS Registry Numbers(s): 31562-40-0 67501-06-8 67734-35-4 79599-55-6 85085-04-7 85085-05-8

$(\text{H}_3\text{C})_3\text{C-S-S-C}(\text{CH}_3)_3$

Molecular Formula: $\text{C}_8\text{H}_{18}\text{S}_2$

Molecular Weight: 178.362

Accurate Mass: 178.08499

Percentage Composition: C 53.87%; H 10.17%; S 35.96%

Physical Description: Oil

Melting Point: Mp -4.95°

Boiling Point: Bp₂₁ 88°

Density: d_4^{20} 0.923

Refractive Index: n_D^{20} 1.4899

Aldrich: 24754-5

Fluka: 34690

Sigma: B1634

>>Derivative: S-Oxide, (S)-form

CAS Registry Number: 60011-16-7

Molecular Formula: $\text{C}_8\text{H}_{18}\text{OS}_2$

Molecular Weight: 194.362

Accurate Mass: 194.079905

Percentage Composition: C 49.44%; H 9.33%; O 8.23%; S 33.00%

Optical Rotation: $[\alpha]_D -63.5$ (c, 1.3 in CH_2Cl_2) (41% ee)

References:

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Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 353A, (*ir*)

Birch, S.F. *et al.*, *J. Inst. Pet.*, 1953, **39**, 206, (*synth*)

Cumper, C.W.N. *et al.*, *J.C.S.(A)*, 1966, 239, (*uv*)

Mikolajczyk, H. *et al.*, *J.A.C.S.*, 1978, **100**, 2510, (*oxide, resoln*)

Kice, J.L. *et al.*, *J.A.C.S.*, 1980, **102**, 4448, (*oxides, pmr*)

Freeman, F. *et al.*, *J.A.C.S.*, 1981, **103**, 6232; 1983, **105**, 4039, (*oxides, synth, pmr, cmr*)

Nemecek, C. *et al.*, *Nouv. J. Chim.*, 1986, **10**, 761, (*oxide, synth*)

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