



>>Entry Name: Bis(3-methylbutyl) sulfide

Synonym(s): 1,1'-Thiobis[3-methylbutane], 9Cl. Di(3-methylbutyl) sulfide. Diisopentyl sulfide. Isoamyl sulfide. Diisoamyl sulfide. Isopentyl sulfide

CAS Registry Number: 544-02-5

$(\text{H}_3\text{C})_2\text{CHCH}_2\text{CH}_2\text{SCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$

Molecular Formula: $\text{C}_{10}\text{H}_{22}\text{S}$

Molecular Weight: 174.35

Accurate Mass: 174.14422

Percentage Composition: C 68.89%; H 12.72%; S 18.39%

Physical Description: Oil

Boiling Point: Bp 216°. Bp₁₄ 98-100°

Density: d_4^{20} 0.823

Refractive Index: n_D^{20} 1.4520

Rare Chemicals Library: S57047-8

>>Derivative: S-Oxide

Synonym(s): Bis(3-methylbutyl) sulfoxide. Diisopentyl sulfoxide

CAS Registry Number: 7726-23-0

Molecular Formula: $\text{C}_{10}\text{H}_{22}\text{OS}$

Molecular Weight: 190.349

Accurate Mass: 190.139135

Percentage Composition: C 63.10%; H 11.65%; O 8.41%; S 16.85%

Physical Description: Needles

Melting Point: Mp 38-40°

Boiling Point: Bp₁₂ 148°

Rare Chemicals Library: S36928-4

>>Derivative: S,S-Dioxide

Synonym(s): Bis(3-methylbutyl) sulfone. Diisoamyl sulfone. Isoamyl sulfone

CAS Registry Number: 2051-06-1

Molecular Formula: $\text{C}_{10}\text{H}_{22}\text{O}_2\text{S}$

Molecular Weight: 206.349

Accurate Mass: 206.13405

Percentage Composition: C 58.21%; H 10.75%; O 15.51%; S 15.54%

Physical Description: Needles

Melting Point: Mp 31°

Boiling Point: Bp 290-293°

Other: PB I05370

References:

Sabatier, P. *et al.*, *C. R. Hebd. Seances Acad. Sci.*, 1910, **150**, 1571, (*synth*)

Wegscheider, R. *et al.*, *Monatsh. Chem.*, 1919, **40**, 329, (*synth*)

Knoll, R., *J. Prakt. Chem.*, 1926, **113**, 45, (*oxide*)

Ayers, G.W. *et al.*, *J.A.C.S.*, 1939, **61**, 84

Horner, L. *et al.*, *Chem. Ber.*, 1958, **91**, 75, (*dioxide*)

Gupta, D. *et al.*, *Anal. Chem. Symp. Ser.*, 1983, **12**, 143, (*ms*)

Benedetti, E. *et al.*, *Spectrochim. Acta A*, 1983, **39**, 57, (*ir, conformn*)