



>>Entry Name: Dibutyl sulfide, 8CI

ENTRY UNDER REVIEW

Synonym(s): 1,1'-Thiobisbutane, 9CI. Butyl sulfide. 5-Thianonane. FEMA 2215

CAS Registry Number: 544-40-1

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

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

Molecular Weight: 146.296

Accurate Mass: 146.11292

Percentage Composition: C 65.68%; H 12.40%; S 21.92%

Use/Importance: Inhibits corrosion of iron in acids. Used in extraction of metals

Physical Description: Liq.

Melting Point: Mp -80°

Boiling Point: Bp 185-185.5°

Solubility: Insol. H_2O , sol. Et_2O

Density: d^{20}_4 0.84

Refractive Index: n^{20}_D 1.4926

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 2220 mg/kg

Aldrich: W22150-3

Fluka: 34840

>>Derivative: S-Oxide

Synonym(s): 1,1'-Sulfinylbisbutane, 9CI. Dibutyl sulfoxide

CAS Registry Number: 2168-93-6

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

Molecular Weight: 162.296

Accurate Mass: 162.107835

Percentage Composition: C 59.21%; H 11.18%; O 9.86%; S 19.76%

Physical Description: Needles

Melting Point: Mp 31°

Boiling Point: Bp₃ 102-105°

Aldrich: B10240-7

>>Derivative: S,S-Dioxide

Synonym(s): 1,1'-Sulfonylbisbutane, 9CI. Dibutyl sulfone

CAS Registry Number: 598-04-9

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

Molecular Weight: 178.295

Accurate Mass: 178.10275

Percentage Composition: C 53.89%; H 10.18%; O 17.95%; S 17.98%

Physical Description: Plates (H_2O)

Melting Point: Mp 44°

Aldrich: B10220-2

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 266C; 879B; 881C, (*ir*)
- Aldrich Library of ^{13}C and ^1H FT NMR Spectra*, 1992, **1**, 428C; 1417B; 1419C, (*nmr*)
- Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 350B, (*ir*)
- Mann, F.G. *et al.*, *J.C.S.*, 1935, 1556, (*synth*)
- Vaughan, W.E. *et al.*, *J.O.C.*, 1942, **7**, 472, (*synth*)
- Aplin, R.T. *et al.*, *J.C.S.(B)*, 1967, 513, (*ms*)
- Hardy, F.E. *et al.*, *J.C.S.(C)*, 1969, 2334, (*dioxide*)
- Calo, V. *et al.*, *Int. J. Sulfur Chem., Part A*, 1971, **1**, 130, (*oxide*)
- Reich, H.J. *et al.*, *Synthesis*, 1978, 299, (*dioxide*)
- Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1979, **17**, 769, (*rev, tox*)
- Fenaroli's Handbook of Flavor Ingredients*, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 96
- Encyclopedia of Food and Color Additives*, (ed. Burdock, G.A.), CRC Press, 1997, 356-357
- Ali, M.H. *et al.*, *Synthesis*, 1997, 764-768, (*oxide*)
- Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, BSM125