



>>Entry Name: Dibutyl disulfide, 9CI

Synonym(s): Butyl disulfide

CAS Registry Number: 629-45-8

Related CAS Registry Numbers(s): 7559-55-9 85085-02-5 85085-03-6

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

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%

Biological Source: Constit. of *Ferula assa-foetida*

Physical Description: Oil

Boiling Point: Bp 226°. Bp₆ 94°

Density: d_4^{20} 0.937

Refractive Index: n_D^{20} 1.4923

Hazard & Toxicity: Fl. p. 93°

Aldrich: B9398-9

Fluka: 34688

Sigma: B1509

>>Derivative: S-Oxide

Synonym(s): S-Butyl 1-butanefulfinthioate

CAS Registry Number: 111698-31-8

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%

Other Data: Known as racemate and as opt. active preparation of unknown opt. purity

>>Derivative: S,S'-Dioxide

Synonym(s): Dibutyl disulfoxide

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

Molecular Weight: 210.361

Accurate Mass: 210.07482

Percentage Composition: C 45.68%; H 8.62%; O 15.21%; S 30.49%

Other Data: Obt. as a mixt. of diastereoisomers; characterised by low temp. cmr

>>Derivative: S,S-Dioxide

Synonym(s): S-Butyl 1-butanefulfonythioate

CAS Registry Number: 1118-40-7

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

Molecular Weight: 210.361

Accurate Mass: 210.07482

Percentage Composition: C 45.68%; H 8.62%; O 15.21%; S 30.49%

Boiling Point: Bp_{0.13} 128-130°

>>Derivative: S,S,S'-Trioxide, (±)-form

Synonym(s): 1-[(Butylsulfinyl)sulfonyl]butane

CAS Registry Number: 78186-29-5

Molecular Formula: $\text{C}_8\text{H}_{18}\text{O}_3\text{S}_2$

Molecular Weight: 226.36

Accurate Mass: 226.069735

Percentage Composition: C 42.45%; H 8.01%; O 21.20%; S 28.33%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 31°