



>>Entry Name: Di-2-propenyl sulfide

ENTRY UNDER REVIEW

Synonym(s): 3,3'-Thiobis-1-propene, 9CI. Thiobis-2-propene. Diallyl sulfide. Allyl sulfide. FEMA 2042

CAS Registry Number: 592-88-1

Type of Compound Code(s): WA4700 XA1645 WI2500 XA1150 XA1650 XA1550 XA1950

$\text{H}_2\text{C}=\text{CHCH}_2\text{SCH}_2\text{CH}=\text{CH}_2$

Molecular Formula: $\text{C}_6\text{H}_{10}\text{S}$

Molecular Weight: 114.211

Accurate Mass: 114.05032

Percentage Composition: C 63.10%; H 8.82%; S 28.08%

Source/Synthesis: Present in *Allium* spp., Japanese horseradish (*Wasabia japonica*) and black mustard (*Brassica nigra*) powder. Formed by hydrol. dec. of cabbage

Use/Importance: Shows bactericidal, fungicidal, antithyroid and antineoplastic props. Antihypercholesterolaemic, antihypertensive agent. Flavouring ingredient

Physical Description: Oil with garlic odour

Boiling Point: Bp 139°. Bp₄ 27-28°

Refractive Index: n_D^{20} 1.4880

Calculated Log P Data: Log P 1.99 (calc)

Hazard & Toxicity: Eye, skin and mucous membrane irritant. LD₅₀ (rat, orl) 2980 mg/kg

Aldrich: A3580-1

Fluka: 32660

Sigma: A5639

>>Derivative: S-Oxide

Synonym(s): 3,3'-Sulfinylbis[1-propene], 9CI. Diallyl sulfoxide

CAS Registry Number: 14180-63-3

Molecular Formula: $\text{C}_6\text{H}_{10}\text{OS}$

Molecular Weight: 130.21

Accurate Mass: 130.045235

Percentage Composition: C 55.35%; H 7.74%; O 12.29%; S 24.63%

Physical Description: Brownish-red liq.

Boiling Point: Bp₇ 107-109°. Bp₃ 98-102°

Density: d_4^{20} 1.026

Refractive Index: n_D^{20} 1.5115

>>Derivative: S,S-Dioxide

Synonym(s): 3,3'-Sulfonylbis[1-propene], 9CI. Diallyl sulfone

CAS Registry Number: 16841-48-8

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_2\text{S}$

Molecular Weight: 146.21

Accurate Mass: 146.04015

Percentage Composition: C 49.29%; H 6.89%; O 21.89%; S 21.93%

Physical Description: Liq.

Boiling Point: Bp₅ 114°. Bp₃ 109°

Density: d_4^{20} 1.122

Refractive Index: n_D^{20} 1.4891

References: