



**>>Entry Name: Phenyl 2-propenyl sulfide**

**Synonym(s):** (2-Propenylthio)benzene, 9Cl. Allyl phenyl sulfide, 8Cl

**CAS Registry Number:** 5296-64-0

PhSCH2CH=CH2

**Molecular Formula:** C<sub>9</sub>H<sub>10</sub>S

**Molecular Weight:** 150.244

**Accurate Mass:** 150.05032

**Percentage Composition:** C 71.95%; H 6.71%; S 21.34%

**Melting Point:** Mp -48°

**Boiling Point:** Bp 221°. Bp<sub>3</sub> 75°. Bp<sub>1.5</sub> 59-60°

**Fluka:** 6060

**Rare Chemicals Library:** S61424-6

**>>Derivative: S-Oxide**

**Synonym(s):** (2-Propenylsulfinyl)benzene, 9Cl. Allyl phenyl sulfoxide

**CAS Registry Number:** 19093-37-9

**Molecular Formula:** C<sub>9</sub>H<sub>10</sub>OS

**Molecular Weight:** 166.243

**Accurate Mass:** 166.045235

**Percentage Composition:** C 65.02%; H 6.06%; O 9.62%; S 19.29%

**Boiling Point:** Bp<sub>0.36</sub> 103-104°

**Density:** d<sub>4</sub><sup>25</sup> 1.1205

**Other Data:** Opt. active form also known. [α]<sub>D</sub><sup>19</sup> +176 (EtOH)

**Fluka:** 6062

**Rare Chemicals Library:** S62021-1

**>>Derivative: S,S-Dioxide**

**Synonym(s):** (2-Propenylsulfonyl)benzene, 9Cl. Allyl phenyl sulfone

**CAS Registry Number:** 16212-05-8

**Molecular Formula:** C<sub>9</sub>H<sub>10</sub>O<sub>2</sub>S

**Molecular Weight:** 182.243

**Accurate Mass:** 182.04015

**Percentage Composition:** C 59.32%; H 5.53%; O 17.56%; S 17.60%

**Boiling Point:** Bp<sub>0.7</sub> 140-145°. Bp<sub>0.5</sub> 110-113°

**Density:** d<sub>4</sub><sup>25</sup> 1.184

**Hazard & Toxicity:** LD<sub>50</sub> (mus, ivn) 320 mg/kg

**Aldrich:** 31771-3

**Fluka:** 6061

**Rare Chemicals Library:** S61425-4

**References:**

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 1580A, (*nmr*)

Tarbell, D.S. *et al.*, *J.A.C.S.*, 1952, **74**, 48, (*synth, ir*)

Bowie, J.H. *et al.*, *J.C.S.(B)*, 1966, 951, (*ms*)

Chmutova, G.A., *Zh. Fiz. Khim.*, 1973, **47**, 2139, (*uv*)

Carlier, P. *et al.*, *Can. J. Chem.*, 1977, **55**, 3190, (*synth, pmr*)

Ohta, H. *et al.*, *Chem. Lett.*, 1984, 205, (*synth*)