



>>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: C₉H₁₀S

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°. Bp₃ 75°. Bp_{1.5} 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: C₉H₁₀OS

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_{0.36} 103-104°

Density: d₄²⁵ 1.1205

Other Data: Opt. active form also known. [α]_D¹⁹ +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: C₉H₁₀O₂S

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_{0.7} 140-145°. Bp_{0.5} 110-113°

Density: d₄²⁵ 1.184

Hazard & Toxicity: LD₅₀ (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*)