



>>Entry Name: (Phenylthio)nitromethane

Synonym(s): [(Nitromethyl)thio]benzene, 9CI. Nitromethyl phenyl sulfide

CAS Registry Number: 60595-16-6

PhSCH₂NO₂

Molecular Formula: C₇H₇NO₂S

Molecular Weight: 169.204

Accurate Mass: 169.019749

Percentage Composition: C 49.69%; H 4.17%; N 8.28%; O 18.91%; S 18.95%

Use/Importance: Synthetic intermed. Homologation reagent. In synth. of α-phenylthio cycloalkanones

Physical Description: Pale yellow oil

Boiling Point: Bp_{0.05} 85-95°

>>Derivative: S,S-Dioxide

Synonym(s): (Nitromethyl)sulfonylbenzene. Nitromethyl phenyl sulfone. (Phenylsulfonyl)nitromethane

CAS Registry Number: 21272-85-5

Molecular Formula: C₇H₇NO₄S

Molecular Weight: 201.203

Accurate Mass: 201.009579

Percentage Composition: C 41.79%; H 3.51%; N 6.96%; O 31.81%; S 15.94%

Physical Description: Needles (hexane)

Melting Point: Mp 78-78.5°

Fluka: 79179

References:

Miyashita, M. *et al.*, *Chem. Comm.*, 1978, 362, (*synth*)

Bordwell, F.G. *et al.*, *J.O.C.*, 1978, **43**, 3101, (*synth*)

Banks, B.J. *et al.*, *Chem. Comm.*, 1984, 670, (*use*)

Barrett, A.G.M. *et al.*, *J.O.C.*, 1987, **52**, 4693, (*synth, use*)

Org. Synth., 1989, **68**, 8, (*synth, ir, pmr*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1990, **15**, 264, (*use*)