



>>Entry Name: 1-Phenyl-2-(phenylthio)ethanone, 9CI

Synonym(s): 2-(Phenylthio)acetophenone, 8CI. ω-Phenylmercaptoacetophenone. Phenacyl phenyl sulfide. Benzoyl(phenylthio)methane

CAS Registry Number: 16222-10-9

PhCOCH₂SPh

Molecular Formula: C₁₄H₁₂OS

Molecular Weight: 228.314

Accurate Mass: 228.060885

Percentage Composition: C 73.65%; H 5.30%; O 7.01%; S 14.04%

Physical Description: Needles (EtOH)

Melting Point: Mp 53-54°

>>Derivative: Phenylhydrazone

Physical Description: Orange needles (MeOH)

Melting Point: Mp 116°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Bright-red needles (EtOH/EtOAc)

Melting Point: Mp 150-150.5°

>>Derivative: S-Oxide

Synonym(s): 1-Phenyl-2-(phenylsulfinyl)ethanone, 9CI. 2-(Phenylsulfinyl)acetophenone, 8CI. Phenacyl phenyl sulfoxide

CAS Registry Number: 6099-23-6

Molecular Formula: C₁₄H₁₂O₂S

Molecular Weight: 244.314

Accurate Mass: 244.0558

Percentage Composition: C 68.83%; H 4.95%; O 13.10%; S 13.12%

Physical Description: Cryst. (C₆H₆/heptane)

Melting Point: Mp 79-80°

>>Derivative: S,S-Dioxide

Synonym(s): 1-Phenyl-2-(phenylsulfonyl)ethanone, 9CI. 2-(Phenylsulfonyl)acetophenone, 8CI. Phenacyl phenyl sulfone

CAS Registry Number: 3406-03-9

Molecular Formula: C₁₄H₁₂O₃S

Molecular Weight: 260.313

Accurate Mass: 260.050715

Percentage Composition: C 64.60%; H 4.65%; O 18.44%; S 12.32%

Physical Description: Cryst.

Melting Point: Mp 96°

Aldrich: 34105-3

Rare Chemicals Library: S59673-6

References:

- Tröger, J. *et al.*, *J. Prakt. Chem.*, 1913, **287**, 289, (*dioxide*)
Kroehnke, F. *et al.*, *J. Prakt. Chem.*, 1960, **11**, 256, (*synth*)
Kenny, W.J. *et al.*, *J.A.C.S.*, 1961, **83**, 4019, (*synth, oxide*)
Griesbaum, K. *et al.*, *J.A.C.S.*, 1963, **85**, 1969, (*ir, pmr, oxide, dioxide*)
Krawiec, M. *et al.*, *Acta Cryst. C*, 1989, **45**, 354, (*dioxide, cryst struct*)
Padmanabham, S. *et al.*, *Bull. Chem. Soc. Jpn.*, 1989, **62**, 1358, (*synth, ir, pmr*)
Satoh, T. *et al.*, *Bull. Chem. Soc. Jpn.*, 1990, **63**, 1266, (*oxide, synth*)
Huang, X. *et al.*, *Synth. Commun.*, 1990, **20**, 2291, (*dioxide, synth*)
Kim, K.S. *et al.*, *Tet. Lett.*, 1990, **31**, 2893, (*oxide, synth*)
Solladie-Cavallo, A. *et al.*, *Tetrahedron*, 1992, **48**, 2453, (*oxide, synth, pmr*)
Katritzky, A.R. *et al.*, *J.O.C.*, 1996, **61**, 7564-7570, (*synth, pmr, cmr*)