



>>Entry Name: 1-(Phenylthio)-2-propanone, 9CI

Synonym(s): (Phenylthio)acetone. Acetonyl phenyl sulfide. Methyl (phenylthio)methyl ketone

CAS Registry Number: 5042-53-5

PhSCH₂COCH₃

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%

Physical Description: Cryst.

Melting Point: Mp 34-35°

Boiling Point: Bp₁₂ 135-137°. Bp₅ 117°

Rare Chemicals Library: S57697-2

>>Derivative: S-Oxide

>>Derivative: S,S-Dioxide

Synonym(s): 1-(Phenylsulfonyl)-2-propanone, 9CI

CAS Registry Number: 5000-44-2

Molecular Formula: C₉H₁₀O₃S

Molecular Weight: 198.242

Accurate Mass: 198.035065

Percentage Composition: C 54.53%; H 5.08%; O 24.21%; S 16.18%

Physical Description: Cryst. (CCl₄)

Melting Point: Mp 52-54° (46-47°)

Rare Chemicals Library: S57705-7

References:

Suter, H. *et al.*, *Annalen*, 1952, **576**, 215, (*synth*)

Ohta, H. *et al.*, *J.O.C.*, 1987, **52**, 2735, (*synth, ir, pmr, ms*)

Gu, X.-P. *et al.*, *J.O.C.*, 1987, **52**, 3192, (*synth, ir, pmr*)

Thomsen, M.W. *et al.*, *J.O.C.*, 1988, **53**, 906, (*synth, pmr, cmr, dioxide*)

Ishibashi, H. *et al.*, *Synth. Commun.*, 1989, **19**, 443, (*synth, pmr*)