



>>Entry Name: 3-(Phenylthio)propanoic acid

CAS Registry Number: 5219-65-8

PhSCH2CH2COOH

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%

Melting Point: Mp 59.5-61°

Boiling Point: Bp₁₀ 184°

pKa Value: pK_a 5.58 (50% EtOH aq.)

>>Derivative: S-Oxide

Synonym(s): 3-(Phenylsulfinyl)propanoic acid, 9CI

CAS Registry Number: 49639-31-8

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. (EtOAc)

Melting Point: Mp 94.5-95.5°

>>Derivative: S,S-Dioxide

Synonym(s): 3-(Phenylsulfonyl)propanoic acid, 9CI

CAS Registry Number: 10154-71-9

Molecular Formula: C₉H₁₀O₄S

Molecular Weight: 214.242

Accurate Mass: 214.02998

Percentage Composition: C 50.46%; H 4.70%; O 29.87%; S 14.97%

Use/Importance: Reagent for 3-carbon homologation

Melting Point: Mp 122.5-123.5°

Aldrich: 25157-7

>>Derivative: Me ester

CAS Registry Number: 22198-59-0

Molecular Formula: C₁₀H₁₂O₂S

Molecular Weight: 196.27

Accurate Mass: 196.0558

Percentage Composition: C 61.20%; H 6.16%; O 16.30%; S 16.34%

Physical Description: Oil

Boiling Point: Bp₂ 108-110°

>>Derivative: Chloride

CAS Registry Number: 51849-21-9

Molecular Formula: C₉H₉ClOS

Molecular Weight: 200.688

Accurate Mass: 200.006262

Percentage Composition: C 53.86%; H 4.52%; Cl 17.67%; O 7.97%; S 15.98%

Physical Description: Liq.

Boiling Point: Bp_{1.8} 126°

>>Derivative: Amide

CAS Registry Number: 97721-47-6

Molecular Formula: C₉H₁₁NOS

Molecular Weight: 181.258

Accurate Mass: 181.056134

Percentage Composition: C 59.64%; H 6.12%; N 7.73%; O 8.83%; S 17.69%

Physical Description: Cryst. (CH₂Cl₂/hexane)

Melting Point: Mp 119°