



**>>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:** Bp<sub>10</sub> 184°

**pKa Value:** p*K*<sub>a</sub> 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:** Bp<sub>2</sub> 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<sub>1.8</sub> 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°