



>>Entry Name: (Phenylsulfonyl)acetic acid

Synonym(s): Methyl phenyl sulfone ω-carboxylic acid

CAS Registry Number: 3959-23-7

PhSO₂CH₂COOH

Molecular Formula: C₈H₈O₄S

Molecular Weight: 200.215

Accurate Mass: 200.01433

Percentage Composition: C 47.99%; H 4.03%; O 31.96%; S 16.02%

Physical Description: Cryst. (CHCl₃/petrol)

Melting Point: Mp 113.5-114°

pKa Value: pK_{a1} 2.51 (25°)

Rare Chemicals Library: S40379-2

>>Derivative: Me ester

CAS Registry Number: 34097-60-4

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%

Physical Description: Oil

Boiling Point: Bp_{0.05} 165°. Bp_{0.01} 145°

Density: d 1.28

Refractive Index: n_D²⁰ 1.5350

>>Derivative: Et ester

CAS Registry Number: 7605-30-3

Molecular Formula: C₁₀H₁₂O₄S

Molecular Weight: 228.268

Accurate Mass: 228.04563

Percentage Composition: C 52.62%; H 5.30%; O 28.04%; S 14.05%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 45°

Rare Chemicals Library: S59687-6

>>Derivative: Chloride

CAS Registry Number: 72263-17-3

Molecular Formula: C₈H₇ClO₃S

Molecular Weight: 218.66

Accurate Mass: 217.980442

Percentage Composition: C 43.94%; H 3.23%; Cl 16.21%; O 21.95%; S 14.66%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 58°

>>Derivative: Amide

CAS Registry Number: 35008-50-5

Molecular Formula: C₈H₉NO₃S

Molecular Weight: 199.23

Accurate Mass: 199.030314

Percentage Composition: C 48.23%; H 4.55%; N 7.03%; O 24.09%; S 16.09%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 156°