



>>Entry Name: [(4-Methylphenyl)thio]acetic acid, 9CI

Synonym(s): (*p*-Tolylthio)acetic acid, 8CI. *p*-Tolylthioglycolic acid

CAS Registry Number: 3996-29-0

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%

Physical Description: Cryst. (hexane/toluene)

Melting Point: Mp 95-97° (88-90°)

pKa Value: pK_a 3.96 (25°, H₂O)

Rare Chemicals Library: S75571-0

>>Derivative: Et ester

CAS Registry Number: 14738-27-3

Molecular Formula: C₁₁H₁₄O₂S

Molecular Weight: 210.296

Accurate Mass: 210.07145

Percentage Composition: C 62.83%; H 6.71%; O 15.22%; S 15.25%

Physical Description: Pale yellow liq.

Boiling Point: Bp₁₄ 157°

>>Derivative: Nitrile

CAS Registry Number: 21681-88-9

Molecular Formula: C₉H₉NS

Molecular Weight: 163.243

Accurate Mass: 163.045569

Percentage Composition: C 66.22%; H 5.56%; N 8.58%; S 19.64%

Boiling Point: Bp₃ 168-170°

>>Derivative: Nitrile, *S,S*-dioxide

Synonym(s): *p*-Toluenesulfonylacetoneitrile. *p*-Tosylacetoneitrile

CAS Registry Number: 5697-44-9

Molecular Formula: C₉H₉NO₂S

Molecular Weight: 195.242

Accurate Mass: 195.035399

Percentage Composition: C 55.37%; H 4.65%; N 7.17%; O 16.39%; S 16.42%

Physical Description: Cryst. (MeOH or C₆H₆)

Melting Point: Mp 149-150°

Rare Chemicals Library: S38293-0

Other: Oakwood 3787

>>Derivative: *S*-Oxide

>>Derivative: *S,S*-Dioxide

Synonym(s): [(4-Methylphenyl)sulfonyl]acetic acid, 9CI. (*p*-Tolylsulfonyl)acetic acid, 8CI

CAS Registry Number: 3937-96-0

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: Cryst. (CH₂Cl₂)

Melting Point: Mp 114-115°

Rare Chemicals Library: S38014-8

Other: Oakwood 3785

References: