



>>Entry Name: 3-Amino-4-methylbenzenesulfonic acid, 9Cl

Synonym(s): 2-Aminotoluene-4-sulfonic acid, 8Cl. *o*-Toluidine-5-sulfonic acid. *o*-Methylaniline-5-sulfonic acid

CAS Registry Number: 618-03-1

Molecular Formula: C₇H₉NO₃S

Molecular Weight: 187.219

Accurate Mass: 187.030314

Percentage Composition: C 44.91%; H 4.85%; N 7.48%; O 25.64%; S 17.13%

Physical Description: Cryst. + 1H₂O

Solubility: Mod. sol. H₂O

pKa Value: p*K*_{a1} 3.63 (25°)

Other Data: Becomes anhyd. over H₂SO₄

Rare Chemicals Library: S51850-6

>>Derivative: Fluoride

CAS Registry Number: 328-86-9

Molecular Formula: C₇H₈FNO₂S

Molecular Weight: 189.21

Accurate Mass: 189.025977

Percentage Composition: C 44.44%; H 4.26%; F 10.04%; N 7.40%; O 16.91%; S 16.95%

Melting Point: Mp 96-97°

Rare Chemicals Library: S67192-4

>>Derivative: Fluoride, *N*-Ac

Molecular Formula: C₉H₁₀FNO₃S

Molecular Weight: 231.247

Accurate Mass: 231.036542

Percentage Composition: C 46.75%; H 4.36%; F 8.22%; N 6.06%; O 20.76%; S 13.87%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 188.5-189.5°

>>Derivative: Chloride, *N*-Ac

CAS Registry Number: 13632-46-7

Molecular Formula: C₉H₁₀ClNO₃S

Molecular Weight: 247.702

Accurate Mass: 247.006991

Percentage Composition: C 43.64%; H 4.07%; Cl 14.31%; N 5.65%; O 19.38%; S 12.95%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 144°

>>Derivative: Chloride, *N*-benzoyl

Molecular Formula: C₁₄H₁₂ClNO₃S

Molecular Weight: 309.772

Accurate Mass: 309.022641

Percentage Composition: C 54.28%; H 3.90%; Cl 11.44%; N 4.52%; O 15.49%; S 10.35%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 196°

>>Derivative: Amide

CAS Registry Number: 6274-28-8

Molecular Formula: C₇H₁₀N₂O₂S

Molecular Weight: 186.234

Accurate Mass: 186.046298

Percentage Composition: C 45.15%; H 5.41%; N 15.04%; O 17.18%; S 17.22%

Melting Point: Mp 176°

Rare Chemicals Library: S18471-3