



>>Entry Name: 5-Amino-2-methylbenzenesulfonic acid, 9Cl

Synonym(s): 4-Aminotoluene-2-sulfonic acid, 8Cl. *p*-Toluidine-3-sulfonic acid. *p*-Methylaniline-3-sulfonic acid

CAS Registry Number: 118-88-7

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: Prisms + 1H₂O

Aldrich: 21156-7

>>Derivative: Fluoride

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%

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 62°

>>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: Needles (C₆H₆)

Melting Point: Mp 120-121°

>>Derivative: Chloride, *N*-Ac

CAS Registry Number: 13632-07-0

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: Prisms (Me₂CO aq.)

Melting Point: Mp 124°

>>Derivative: Amide

CAS Registry Number: 6973-09-7

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%

Physical Description: Needles or plates

Melting Point: Mp 164°

>>Derivative: Amide, *N*-Ac

Molecular Formula: C₉H₁₂N₂O₃S

Molecular Weight: 228.271

Accurate Mass: 228.056863

Percentage Composition: C 47.36%; H 5.30%; N 12.27%; O 21.03%; S 14.05%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 242°