



>>Entry Name: 3-Aminobenzenesulfonic acid, 9CI
Synonym(s): Aniline-*m*-sulfonic acid. Metanilic acid

CAS Registry Number: 121-47-1
Related CAS Registry Numbers(s): 1126-34-7

Molecular Formula: C₆H₇NO₃S
Molecular Weight: 173.192
Accurate Mass: 173.014664
Percentage Composition: C 41.61%; H 4.07%; N 8.09%; O 27.71%; S 18.51%
Physical Description: Cryst. + 1½ H₂O
pKa Value: pK_a 3.74 (25°)
Hazard & Toxicity: Eye irritant

Aldrich: 16579-4
Fluka: 6998
Sigma: A6956

>>Derivative: Fluoride

CAS Registry Number: 3887-48-7
Molecular Formula: C₆H₆FNO₂S
Molecular Weight: 175.183
Accurate Mass: 175.010327
Percentage Composition: C 41.14%; H 3.45%; F 10.84%; N 8.00%; O 18.27%; S 18.30%
Physical Description: Monohydrate
Melting Point: Mp 200 dec.° (as hydrochloride, hydrate)
Other Data: CAS no. refers to hydrochloride

>>Derivative: Amide

CAS Registry Number: 98-18-0
Molecular Formula: C₆H₈N₂O₂S
Molecular Weight: 172.207
Accurate Mass: 172.030648
Percentage Composition: C 41.85%; H 4.68%; N 16.27%; O 18.58%; S 18.62%
Physical Description: Cryst.
Melting Point: Mp 142°

>>Derivative: Amide, *N*-butyl

CAS Registry Number: 143173-93-7
Molecular Formula: C₁₀H₁₆N₂O₂S
Molecular Weight: 228.315
Accurate Mass: 228.093248
Percentage Composition: C 52.61%; H 7.06%; N 12.27%; O 14.02%; S 14.04%
Melting Point: Mp 73-77°
Aldrich: 38747-9

>>Derivative: *N*-Me

CAS Registry Number: 71794-43-9
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: Needles (H₂O)
Melting Point: Mp 285-290 dec.°