



-->Entry Name: 3-Aminobenzenesulfonic acid, 90
Synonym(s): Aniline-*m*-sulfonic acid. Metanilic acid

CAS Registry Number: 121-47-1

Related CAS Registry Number(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: A0956

-->Derivative: Fluoride

CAS Registry Number: 3887-48-7
Molecular Formula: C₆H₄FN₂O₃S
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: C₆H₆N₂O₃S
Molecular Weight: 172.207
Accurate Mass: 172.03648
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: C₁₀H₁₂N₂O₃S
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: 187.03014
Percentage Composition: C 44.91%; H 4.85%; N 7.48%; O 25.64%; S 17.13%
Physical Description: Nodules (H₂O)
Melting Point: Mp 285-290 dec.°

-->Derivative: N-Et

Molecular Formula: C₈H₁₁NO₃S
Molecular Weight: 201.246
Accurate Mass: 201.045964
Percentage Composition: C 47.75%; H 5.51%; N 6.96%; O 23.85%; S 15.93%
Physical Description: Cryst. (H₂O)
Melting Point: Mp 294 dec.°

-->Derivative: N,N-Di-Et

CAS Registry Number: 97-20-1
Molecular Formula: C₁₀H₁₃NO₃S
Molecular Weight: 229.299
Accurate Mass: 229.07264
Percentage Composition: C 52.38%; H 6.59%; N 6.11%; O 20.93%; S 13.98%
Physical Description: Cryst.
Melting Point: Mp 270 dec.°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 518B, (*tr. fluoride*)
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Jacobs, D. *et al.*, *J.A.C.S.*, 1917, **39**, 2428
Shirodkar, G.V. *et al.*, *J. Indian Chem. Soc.*, 1940, **17**, 443, (*deriv*)
Nakajima, T., *Bull. Chem. Soc. Jpn.*, 1969, **42**, 2706, (*deriv*)
Lally, J.M. *et al.*, *Chem. Comm.*, 1987, 1571, (*propyl*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, SNC000