



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

Synonym(s): 4-Chlorometanilic acid, 8Cl. 2-Chloroaniline-5-sulfonic acid

CAS Registry Number: 98-36-2

Molecular Formula: C₆H₆ClNO₃S

Molecular Weight: 207.637

Accurate Mass: 206.975691

Percentage Composition: C 34.71%; H 2.91%; Cl 17.07%; N 6.75%; O 23.12%; S 15.44%

Physical Description: Needles (H₂O)

>>Derivative: Fluoride

CAS Registry Number: 368-72-9

Molecular Formula: C₆H₅ClFNO₂S

Molecular Weight: 209.628

Accurate Mass: 208.971354

Percentage Composition: C 34.38%; H 2.40%; Cl 16.91%; F 9.06%; N 6.68%; O 15.26%; S 15.30%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 74-75° (62-64°)

Aldrich: 14297-2

>>Derivative: Amide

CAS Registry Number: 29092-34-0

Molecular Formula: C₆H₇ClN₂O₂S

Molecular Weight: 206.652

Accurate Mass: 205.991675

Percentage Composition: C 34.87%; H 3.41%; Cl 17.16%; N 13.56%; O 15.48%; S 15.52%

Melting Point: Mp 168-170°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 524A, (*ir*)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 843A, (*nmr*)

Fischer, P., *Ber.*, 1891, **24**, 3185, (*synth*)

Jackman, G.B. *et al.*, *J. Pharm. Pharmacol.*, 1960, **12**, 648, (*amide*)

Maruyama, T. *et al.*, *CA*, 1961, **55**, 11855a, (*fluoride*)

Biernacki, W., *Pol. J. Chem. (Rocz. Chem.)*, 1972, **46**, 613, (*synth*)