



>>Entry Name: 4-Chloro-3-nitrobenzenesulfonic acid, 9Cl, 8Cl

CAS Registry Number: 121-18-6

Related CAS Registry Numbers(s): 17691-19-9

Molecular Formula: C₆H₄ClNO₅S

Molecular Weight: 237.62

Accurate Mass: 236.949871

Percentage Composition: C 30.33%; H 1.70%; Cl 14.92%; N 5.89%; O 33.67%; S 13.49%

Physical Description: Cryst. + H₂O

>>Derivative: Chloride

CAS Registry Number: 97-08-5

Molecular Formula: C₆H₃Cl₂NO₄S

Molecular Weight: 256.065

Accurate Mass: 254.915983

Percentage Composition: C 28.14%; H 1.18%; Cl 27.69%; N 5.47%; O 24.99%; S 12.52%

Physical Description: Cryst.

Melting Point: Mp 40-41° (60-61°)

Aldrich: C5940-8

>>Derivative: Amide

CAS Registry Number: 97-09-6

Molecular Formula: C₆H₅ClN₂O₄S

Molecular Weight: 236.635

Accurate Mass: 235.965855

Percentage Composition: C 30.45%; H 2.13%; Cl 14.98%; N 11.84%; O 27.04%; S 13.55%

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 175-176°

Rare Chemicals Library: S38714-2

References:

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

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **2**, 1624B, (*nmr*)

Fischer, E., *Ber.*, 1891, **24**, 3187, (*synth*)

Miller, J. *et al.*, *Chem. Ind. (London)*, 1954, 1457, (*use*)

Lynch, D.C. *et al.*, *Synth. Commun.*, 1997, **27**, 897-905, (*chloride*)