



>>Entry Name: Aminomethanesulfonic acid, 9CI

CAS Registry Number: 13881-91-9

H2NCH2SO3H

Molecular Formula: CH5NO3S

Molecular Weight: 111.121

Accurate Mass: 110.999014

Percentage Composition: C 10.81%; H 4.54%; N 12.60%; O 43.19%; S 28.86%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 184-185 dec.°

Aldrich: 12744-2

Fluka: 8398

Sigma: A0927

>>Derivative: *N*-Me

Synonym(s): (Methylamino)methanesulfonic acid, 9CI

CAS Registry Number: 23592-45-2

Molecular Formula: C2H7NO3S

Molecular Weight: 125.148

Accurate Mass: 125.014664

Percentage Composition: C 19.19%; H 5.64%; N 11.19%; O 38.35%; S 25.62%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 165.5-167.5 dec.°

>>Derivative: *N,N*-Di-Me

Synonym(s): (Dimethylamino)methanesulfonic acid, 9CI

CAS Registry Number: 68507-34-6

Molecular Formula: C3H9NO3S

Molecular Weight: 139.175

Accurate Mass: 139.030314

Percentage Composition: C 25.89%; H 6.52%; N 10.06%; O 34.49%; S 23.04%

Physical Description: Cryst.

Melting Point: Mp 155°

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **1**, 889D, (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 791D, (*nmr*)
Backer, H.J. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1933, **52**, 454, (*derivs*)
Hartough, H.D. *et al.*, *J.A.C.S.*, 1950, **72**, 1572, (*synth*)
Lacoste, R.G. *et al.*, *J.A.C.S.*, 1955, **77**, 5512, (*synth*)
Fujii, A. *et al.*, *J. Med. Chem.*, 1975, **18**, 502, (*synth, props*)
Boehme, H. *et al.*, *Chem. Ber.*, 1978, **111**, 3294, (*deriv*)
Cassidei, L. *et al.*, *J. Magn. Reson.*, 1985, **62**, 529, (*³³S nmr*)
King, J.F. *et al.*, *Phosphorus Sulfur Relat. Elem.*, 1985, **25**, 11, (*deriv*)