



>>Entry Name: 1-Pentanesulfonic acid, 9CI

Synonym(s): 1-Pentylsulfonic acid

CAS Registry Number: 35452-30-3

$\text{H}_3\text{C}(\text{CH}_2)_3\text{CH}_2\text{SO}_3\text{H}$

Molecular Formula: $\text{C}_5\text{H}_{12}\text{O}_3\text{S}$

Molecular Weight: 152.214

Accurate Mass: 152.050715

Percentage Composition: C 39.45%; H 7.95%; O 31.53%; S 21.07%

Physical Description: Liq.

Melting Point: Mp 15.9°

Boiling Point: Bp₁ 163°

Density: d₄²⁵ 1.226

>>Derivative: Na salt

CAS Registry Number: 22767-49-3

Use/Importance: Ion-pairing reagent used in hplc inc. analysis of peptides and proteins

Melting Point: Mp 300°

Aldrich: 39704-0

Fluka: 76952

Sigma: P2441

Supelco: R42-2833

>>Derivative: Me ester

CAS Registry Number: 2697-53-2

Molecular Formula: $\text{C}_6\text{H}_{14}\text{O}_3\text{S}$

Molecular Weight: 166.241

Accurate Mass: 166.066365

Percentage Composition: C 43.35%; H 8.49%; O 28.87%; S 19.29%

Physical Description: Liq.

Boiling Point: Bp_{2.2} 96.4°. Bp_{0.3} 80°

Density: d₄²⁰ 1.087

Refractive Index: n_D²⁰ 1.4339

>>Derivative: Et ester

CAS Registry Number: 91284-44-5

Molecular Formula: $\text{C}_7\text{H}_{16}\text{O}_3\text{S}$

Molecular Weight: 180.268

Accurate Mass: 180.082015

Percentage Composition: C 46.64%; H 8.95%; O 26.63%; S 17.79%

Boiling Point: Bp₆ 102°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1429A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 886C, (*ir*)

Vivian, D.L. *et al.*, *J.A.C.S.*, 1935, **57**, 2559, (*synth*)

Truce, W.E. *et al.*, *J.O.C.*, 1967, **32**, 308, (*synth*)

Hancock, W.S. *et al.*, *J. Chromatogr.*, 1978, **161**, 291, (*use*)

Johnson, T.J. *et al.*, *Tetrahedron*, 1978, **34**, 547, (*synth*)

Bidlingmeyer, B.A. *et al.*, *Adv. Chromatogr. (Houston) 19th 1984*, 1979, **14**, 435; *CA*, **91**, 217413a, (*use*)

Ninomiya, S.-I. *et al.*, *Chem. Pharm. Bull.*, 1984, **32**, 1326, (*synth*)

Costanzo, S.J., *J. Chromatogr.*, 1984, **314**, 402, (*use*)