



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

Synonym(s): 1-Decylsulfonic acid

CAS Registry Number: 13419-61-9

Related CAS Registry Numbers(s): 20283-21-0

$\text{H}_3\text{C}(\text{CH}_2)_8\text{CH}_2\text{SO}_3\text{H}$

Molecular Formula: $\text{C}_{10}\text{H}_{22}\text{O}_3\text{S}$

Molecular Weight: 222.348

Accurate Mass: 222.128965

Percentage Composition: C 54.02%; H 9.97%; O 21.59%; S 14.42%

Aldrich: 22157-0

Fluka: 30635

Sigma: D3147

>>Derivative: Na salt

Use/Importance: Ion-pairing reagent used in hplc

Physical Description: Sl. hygroscopic cryst. (EtOH)

Other Data: Forms a quarter-hydrate and a hemihydrate

>>Derivative: Me ester

CAS Registry Number: 67779-44-6

Molecular Formula: $\text{C}_{11}\text{H}_{24}\text{O}_3\text{S}$

Molecular Weight: 236.375

Accurate Mass: 236.144615

Percentage Composition: C 55.89%; H 10.23%; O 20.31%; S 13.57%

Physical Description: Liq.

Boiling Point: $\text{Bp}_{0.3}$ 120°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 887C, (*ir*)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 790A, (*nmr*)

Reed, R.M. *et al.*, *J.A.C.S.*, 1935, **57**, 570, (*synth*)

Jensen, L.H. *et al.*, *J.A.C.S.*, 1944, **66**, 1946; 1946, **68**, 2730, (*cryst struct, salt*)

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

Walker, T.A. *et al.*, *J. Liq. Chromatogr.*, 1987, **10**, 161, (*use*)