



>>Entry Name: 1-Propanesulfonic acid, 9Cl

CAS Registry Number: 5284-66-2

H3CCH2CH2SO3H

Molecular Formula: C3H8O3S

Molecular Weight: 124.16

Accurate Mass: 124.019415

Percentage Composition: C 29.02%; H 6.49%; O 38.66%; S 25.83%

pKa Value: pK_a 6.2

>>Derivative: Chloride

CAS Registry Number: 10147-36-1

Molecular Formula: C3H7ClO2S

Molecular Weight: 142.606

Accurate Mass: 141.985527

Percentage Composition: C 25.27%; H 4.95%; Cl 24.86%; O 22.44%; S 22.49%

Boiling Point: Bp 180° dec.. Bp₁₃ 77.3-78°

Aldrich: 40440-3

Fluka: 81810

>>Derivative: Amide

CAS Registry Number: 24243-71-8

Molecular Formula: C3H9NO2S

Molecular Weight: 123.176

Accurate Mass: 123.035399

Percentage Composition: C 29.25%; H 7.36%; N 11.37%; O 25.98%; S 26.03%

Physical Description: Prisms (Et₂O)

Melting Point: Mp 52°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1447B, (*nmr*)

Wagner, F.C. *et al.*, *J.A.C.S.*, 1931, **53**, 3411, (*props*)

Latimer, P.H. *et al.*, *J.O.C.*, 1940, **5**, 25, (*synth*)

Pantlitschko, M. *et al.*, *Monatsh. Chem.*, 1958, **89**, 285, (*synth*)