



>>Entry Name: 2-Propanesulfonic acid, 9Cl

Synonym(s): Isopropylsulfonic acid

CAS Registry Number: 14159-48-9

$(\text{H}_3\text{C})_2\text{CHSO}_3\text{H}$

Molecular Formula: $\text{C}_3\text{H}_8\text{O}_3\text{S}$

Molecular Weight: 124.16

Accurate Mass: 124.019415

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

Physical Description: Liq.

Melting Point: Mp -37°

Boiling Point: Bp_{1.4} 159°

Density: d_4^{25} 1.187

Refractive Index: n_D^{20} 1.4332

>>Derivative: Chloride

CAS Registry Number: 10147-37-2

Molecular Formula: $\text{C}_3\text{H}_7\text{ClO}_2\text{S}$

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%

Use/Importance: Used in dehydroxylation

Physical Description: Oil

Boiling Point: Bp₁₈ 79°

Aldrich: 24270-5

Fluka: 81812

>>Derivative: Amide

Molecular Formula: $\text{C}_3\text{H}_9\text{NO}_2\text{S}$

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: Cryst. (Et_2O /petrol)

Melting Point: Mp 60°

References:

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

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 900D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 835B, (*ir*)

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

Zuffanti, S. *et al.*, *J.A.C.S.*, 1940, **62**, 1044, (*synth*)

Lowe, O.G., *J.O.C.*, 1976, **41**, 2061, (*synth*)

Hua, D.H. *et al.*, *J.A.C.S.*, 1985, **107**, 14088, (*use, chloride*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1988, **13**, 153, (*use*)