



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

Synonym(s): 1-Octylsulfonic acid

CAS Registry Number: 3944-72-7

$\text{H}_3\text{C}(\text{CH}_2)_6\text{CH}_2\text{SO}_3\text{H}$

Molecular Formula: $\text{C}_8\text{H}_{18}\text{O}_3\text{S}$

Molecular Weight: 194.294

Accurate Mass: 194.097665

Percentage Composition: C 49.45%; H 9.34%; O 24.70%; S 16.50%

>>Derivative: Na salt

CAS Registry Number: 5324-84-5

Use/Importance: Ion-pairing reagent used in hplc

Physical Description: Hygroscopic cryst. (EtOH)

Melting Point: Mp 300°

Aldrich: 22156-2

Fluka: 74885

Sigma: O6507

Supelco: R42-2830

>>Derivative: Me ester

CAS Registry Number: 10307-28-5

Molecular Formula: $\text{C}_9\text{H}_{20}\text{O}_3\text{S}$

Molecular Weight: 208.321

Accurate Mass: 208.113315

Percentage Composition: C 51.89%; H 9.68%; O 23.04%; S 15.39%

Physical Description: Liq.

Boiling Point: Bp_{0.3} 103°

>>Derivative: Et ester

CAS Registry Number: 5455-54-9

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%

Physical Description: Liq.

Boiling Point: Bp₁ 113°

Density: d₄²⁵ 1.0009

Refractive Index: n_D²⁵ 1.4382

>>Derivative: Chloride

CAS Registry Number: 7795-95-1

Molecular Formula: $\text{C}_8\text{H}_{17}\text{ClO}_2\text{S}$

Molecular Weight: 212.74

Accurate Mass: 212.063777

Percentage Composition: C 45.17%; H 8.05%; Cl 16.66%; O 15.04%; S 15.07%

Melting Point: Mp 15.5-16.5°

Boiling Point: Bp₁ 94°

Density: d₄²⁵ 1.457

Refractive Index: n_D²⁰ 1.4591

Aldrich: 37419-9

Fluka: 74883

References: