



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

Synonym(s): Cetylsulfonic acid

CAS Registry Number: 6140-88-1

Related CAS Registry Numbers(s): 15015-81-3

$\text{H}_3\text{C}(\text{CH}_2)_{15}\text{SO}_3\text{H}$

Molecular Formula: $\text{C}_{16}\text{H}_{34}\text{O}_3\text{S}$

Molecular Weight: 306.509

Accurate Mass: 306.222865

Percentage Composition: C 62.70%; H 11.18%; O 15.66%; S 10.46%

Physical Description: Cryst. (petrol)

Melting Point: Mp 72.5-73°

>>Derivative: S-Benzylthiuronium salt

Melting Point: Mp 122-123°

>>Derivative: Me ester

CAS Registry Number: 4230-15-3

Molecular Formula: $\text{C}_{17}\text{H}_{36}\text{O}_3\text{S}$

Molecular Weight: 320.536

Accurate Mass: 320.238515

Percentage Composition: C 63.70%; H 11.32%; O 14.97%; S 10.00%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 47.7-47.9°

>>Derivative: Chloride

CAS Registry Number: 38775-38-1

Molecular Formula: $\text{C}_{16}\text{H}_{33}\text{ClO}_2\text{S}$

Molecular Weight: 324.954

Accurate Mass: 324.188977

Percentage Composition: C 59.14%; H 10.24%; Cl 10.91%; O 9.85%; S 9.87%

Physical Description: Cryst. (petrol)

Melting Point: Mp 56.5-57.5°

References:

Stowell, J.S. *et al.*, *J.O.C.*, 1962, **27**, 2853, (*synth*)

U.S. Pat., 1970, 3 518 299; *CA*, **73**, 98388, (*synth*)

Barbero, M. *et al.*, *Synthesis*, 1989, 957, (*chloride*)