



>>Entry Name: 2-(Octylthio)ethanol, 9CI

Synonym(s): 2-Hydroxyethyl octyl sulfide

CAS Registry Number: 3547-33-9

$\text{H}_3\text{C}(\text{CH}_2)_7\text{SCH}_2\text{CH}_2\text{OH}$

Molecular Formula: $\text{C}_{10}\text{H}_{22}\text{OS}$

Molecular Weight: 190.349

Accurate Mass: 190.139135

Percentage Composition: C 63.10%; H 11.65%; O 8.41%; S 16.85%

Use/Importance: Insect repellent. Low acute mammalian toxicity

Physical Description: Pale amber liq.

Melting Point: Mp 0°

Boiling Point: Bp_{0.1} 98°

Solubility: Sl. sol. H_2O ; misc. most org. solvs.

Density: d_4^{20} 0.93

Rare Chemicals Library: S36915-2

>>Derivative: S-Oxide, (±)-form

Synonym(s): 2-(Octylsulfinyl) ethanol. 2-Hydroxyethyl octyl sulfoxide

CAS Registry Number: 7305-30-8

Molecular Formula: $\text{C}_{10}\text{H}_{22}\text{O}_2\text{S}$

Molecular Weight: 206.349

Accurate Mass: 206.13405

Percentage Composition: C 58.21%; H 10.75%; O 15.51%; S 15.54%

Use/Importance: Zwitterionic detergent

Melting Point: Mp 54°

>>Derivative: S,S-Dioxide

Synonym(s): 2-(Octylsulfonyl) ethanol. 2-Hydroxyethyl octyl sulfone

CAS Registry Number: 20466-47-1

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%

Melting Point: Mp 73°

References:

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Kabachnik, M.I. *et al.*, *Zh. Obshch. Khim.*, 1963, **33**, 1941, (*synth*)

Novitskaya, N.N. *et al.*, *Neftekhimiya*, 1968, **8**, 770; *CA*, **70**, 46756, (*synth, deriv*)

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