



>>Entry Name: 1-Octanol, 9CI

Synonym(s): *n*-Octyl alcohol. Caprylic alcohol. FEMA 2800

CAS Registry Number: 111-87-5

Extra CAS Registry Numbers(s): 29063-28-3

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

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

Molecular Weight: 130.23

Accurate Mass: 130.135765

Percentage Composition: C 73.78%; H 13.93%; O 12.29%

Biological Source: Occurs in the form of esters in some essential oils

Use/Importance: Diverse use including the manuf. of perfumes, insecticides and esters. Antifoaming agent. Flavouring agent

Physical Description: Liq. with penetrating aromatic odour

Melting Point: Mp -16.7°

Boiling Point: Bp 194.45° . Bp₁₉ 98°

Density: d_4^{20} 0.827

Refractive Index: n_D^{20} 1.4295

Hazard & Toxicity: Skin irritant. LD₅₀ (mus, orl) 1790 mg/kg

Aldrich: 47232-8

Fluka: 74852

Sigma: O4500

Supelco: R42-1820

>>Derivative: Sulfate, Na salt

Synonym(s): Sodium octyl sulfate

CAS Registry Number: 142-31-4

Use/Importance: Detergent

Melting Point: Mp 195 dec.°

Aldrich: 39025-9

Fluka: 75074

Sigma: O4003

>>Derivative: *O*-[α -D-Arabinofuranosyl-(1 $\rightarrow$ 6)- β -D-glucopyranoside]

CAS Registry Number: 183994-73-2

Molecular Formula: $\text{C}_{19}\text{H}_{36}\text{O}_{10}$

Molecular Weight: 424.487

Accurate Mass: 424.23085

Percentage Composition: C 53.76%; H 8.55%; O 37.69%

Biological Source: Constit. of *Circaea lutetiana* ssp. *canadensis*

Physical Description: Waxy semisolid

Optical Rotation: $[\alpha]_D^{26} -75$ (c, 0.6 in MeOH)

>>Derivative: *O*-[α -L-Arabinopyranosyl-(1 $\rightarrow$ 6)- β -D-glucopyranoside]

Synonym(s): Rhodiooctanoside

CAS Registry Number: 168288-07-1

Molecular Formula: $\text{C}_{19}\text{H}_{36}\text{O}_{10}$

Molecular Weight: 424.487

Accurate Mass: 424.23085

Percentage Composition: C 53.76%; H 8.55%; O 37.69%

Biological Source: Constit. of *Rhodiola quadrifida*

Physical Description: Amorph. powder

Optical Rotation: $[\alpha]_D^{24} -29.2$ (c, 0.8 in MeOH)

>>Derivative: Formyl

Synonym(s): Octyl formate. FEMA 2809

CAS Registry Number: 112-32-3