



>>Entry Name: 1-Dodecanol

ENTRY UNDER REVIEW

Synonym(s): Dodecyl alcohol. Lauryl alcohol. FEMA 2617

CAS Registry Number: 112-53-8

Related CAS Registry Numbers(s): 27342-88-7

Type of Compound Code(s): WI5000 WI4000 WI3500 WE9000 WI7000 WI3200 WE9000 WE9999 VA0100

$\text{H}_3\text{C}(\text{CH}_2)_{10}\text{CH}_2\text{OH}$

Molecular Formula:  $\text{C}_{12}\text{H}_{26}\text{O}$

Molecular Weight: 186.337

Accurate Mass: 186.198365

Percentage Composition: C 77.35%; H 14.06%; O 8.59%

Biological Source: Isol. from plant sources, eg. oil of *Furcraea gigantea*, apple and banana. Occurs also as ester

Use/Importance: Used in perfumery. Sulfuric esters are used as wetting agents and detergents. Flavouring agent

Physical Description: Cryst. (EtOH aq.) with fatty, waxy flavour

Melting Point: Mp 24°. Mp 26°

Boiling Point: Bp 260-262°. Bp<sub>18</sub> 145-148°

Hazard & Toxicity: Severe skin irritant. LD<sub>50</sub> (rat, orl) ca. 13000 mg/kg

Aldrich: 12679-9

Fluka: 44110

Sigma: L5375

>>Derivative: *O*-[ $\alpha$ -L-Rhamnopyranosyl-(1→3)-2-*O*-acetyl- $\alpha$ -L-rhamnopyranosyl-(1→3)-4-*O*-acetyl- $\alpha$ -L-rhamnopyranosyl-(1→4)- $\alpha$ -L-rhamnopyranoside]

CAS Registry Number: 115547-17-6

Type of Compound Code(s): VA0100 VE9300

Molecular Formula:  $\text{C}_{40}\text{H}_{70}\text{O}_{19}$

Molecular Weight: 854.982

Accurate Mass: 854.451135

Percentage Composition: C 56.19%; H 8.25%; O 35.55%

Biological Source: Constit. of *Cleistopholis glauca*

>>Derivative: *O*-[ $\alpha$ -L-Rhamnopyranosyl-(1→3)-2,4-di-*O*-acetyl- $\alpha$ -L-rhamnopyranosyl-(1→3)-4-*O*-acetyl- $\alpha$ -L-rhamnopyranosyl-(1→4)- $\alpha$ -L-rhamnopyranoside]

Synonym(s): Cleistetroside 4

CAS Registry Number: 115547-18-7

Type of Compound Code(s): VA0100 VE9300

Molecular Formula:  $\text{C}_{42}\text{H}_{72}\text{O}_{20}$

Molecular Weight: 897.019

Accurate Mass: 896.4617

Percentage Composition: C 56.24%; H 8.09%; O 35.67%

Biological Source: Constit. of *Cleistopholis glauca*

Physical Description: Gummy solid

Melting Point: Mp 107-109°

Optical Rotation:  $[\alpha]_{\text{D}}^{21} -79.5$  (c, 0.18 in MeOH)

>>Derivative: *O*-[2-*O*-Acetyl- $\alpha$ -L-rhamnopyranosyl-(1→3)-2,4-di-*O*-acetyl- $\alpha$ -L-rhamnopyranosyl-(1→3)-4-*O*-acetyl- $\alpha$ -L-rhamnopyranosyl-(1→4)- $\alpha$ -L-rhamnopyranoside]

Synonym(s): Cleistetroside 3

CAS Registry Number: 115547-20-1

Type of Compound Code(s): VE9300 VA0100

Molecular Formula:  $\text{C}_{44}\text{H}_{74}\text{O}_{21}$

Molecular Weight: 939.056

Accurate Mass: 938.472265

Percentage Composition: C 56.28%; H 7.94%; O 35.78%

Biological Source: Constit. of *Cleistopholis glauca*

Physical Description: Gummy solid

Melting Point: Mp 98-100°

Optical Rotation:  $[\alpha]_{\text{D}}^{23} -54.7$  (c, 0.26 in MeOH)