



Formula: C<sub>20</sub>H<sub>36</sub>O<sub>2</sub>

MW: 308.5

CAS: 515-03-7

MDL: MFCD03225426

TNP: TNP00106

(1R,2R,8AS)-DECAHYDRO-1-(3-HYDROXY-3-METHYL-4-PENTENYL)-2,5,5,8A-TETRAMETHYL-2-NAPHTHOL; SCLAREOL; (13r)-labd-14-ene-13-diol;  
(1r-(1- $\alpha$ (r\*),2- $\beta$ ,4a- $\beta$ ,8a- $\alpha$ ))-thyl;  
.alpha.-ethenyldecahydro-2-hydroxy-.alpha.,2,5,5,8a-pentamethyl-,[1R-[1.alpha.(R\*),2



LogP: 5.09

LogS:

Acceptors: 2

Donors: 2

Rotation Bonds: 3

Chiral Centers: 5

N+O: 2

LIPINSKY: 4

Info: A ditertiary, bicyclic alcohol of the formula C<sub>20</sub>H<sub>36</sub>O<sub>2</sub> produced by the hydrocarbon solvent extraction of the plant *Salvia sclarea*

IUPAC: 2-((3S)-3-hydroxy-3-methylpent-4-enyl)(1S,6S,2R,3R)-1,3,7,7-tetramethylbicyclo[4.4.0]decan-3-ol

Smiles: C1[C@@H]2([C]([C@H]([C@@](C1)(O)C)CC[C@@](C=C)(O)C)(CCC[C@]2(C)C)C

REFERENCE: # ^ Good Scents Company # ^ Dimas, Kostas; Kokkinopoulos, Dimitrios; Demetzos, Costas; Vaos, Basilios; Marselos, Marios; Malamas, Mixalis; Tzavaras, Theodoros (1999). "The effect of sclareol on growth and cell cycle progression of human leukemic cell lines". *Leukemia Research* 23 (3): 217-234. # ^ K. Dimas (2007). "Sclareol induces apoptosis in human HCT116 colon cancer cells in vitro and suppression of HCT116 tumor growth in immunodeficient mice". *Apoptosis* 12 (4): 685-694. doi:10.1007/s10495-006-0026-8. <http://www.ingentaconnect.com/content/klu/appt/2007/00000012/00000004/00000026>.

SOURCE: Sclareol is a fragrant chemical compound found in clary sage (*Salvia sclarea*), from which it derives its name. It is classified as a bicyclic diterpene alcohol. It is an amber colored solid with a sweet, balsamic scent.[1]

ACTIVITY: Sclareol is used as a fragrance in cosmetics and perfumes and as flavoring in food. Sclareol and other similar substances may be prepared from sclareolide. Sclareol is also able to kill human leukemic cells and colon cancer cells by apoptosis.[2][3]

Specification: Organics; Natural Plant Extract; Flavors & Fragrances Sclareol Chemical Properties:

mp 95-100 C(lit.) bp 218-220 C19 mm Hg(lit.) alpha -13