



Formula: C<sub>10</sub>H<sub>20</sub>O

MW: 156.27

CAS: 106-22-9

MDL: MFCD00002935

TNP: TNP00396

2,6-DIMETHYL-2-OCTEN-8-OL; 6-OCTEN-1-OL, 3,7-DIMETHYL;  
3,7-DIMETHYL-6-OCTEN-1-OL; 3,7-DIMETHYL-OCT-6-EN-1-OL; (+/-)-CITRONELLOL;  
CITRONELLOL; CITRONELLOL PRIME; CITRONELLOL EXTRA



LogP: 3.87

LogS: -4.58

Acceptors: 1

Donors: 1

Rotation Bonds: 6

Chiral Centers: 1

N+O: 1

LIPINSKY: 4

Oil: LIQUID

Info: Citronellol 95%

IUPAC: 3,7-dimethyloct-6-en-1-ol

Smiles: CC(=CCCC(CCO)C)C

SOURCE: L-form is a constituent of rose and geranium oils. D-form occurs in Ceylon and Java citronella oils.

Specification: Acyclic Monoterpenes; Biochemistry; Terpenes; Alphabetical Listings; C-D; Flavors and Fragrances Citronellol Chemical Properties:

mp 77-83 C(lit.) bp 225 C(lit.) density 0.857 g/mL at 25 C(lit.) vapor density 5.4 (vs air) vapor pressure ~0.02 mm Hg ( 25 C) FEMA 2309 refractive index n<sub>20/D</sub> 1.456(lit.) Fp 209 F storage temp. 2-8C Water Solubility SLIGHTLY SOLUBLE Merck 14,2330 BRN 1721507

Stability:Stable. Incompatible with oxidizing agents. CAS DataBase Reference106-22-9(CAS DataBase Reference) NIST Chemistry Reference6-Octen-1-ol, 3,7-dimethyl-(106-22-9) EPA Substance Registry System6-Octen-1-ol, 3,7-dimethyl-(106-22-9) Safety Information Hazard Codes Xi Risk Statements 36/37/38 Safety Statements 26-36-24/25 WGK Germany 1 RTECS RH3400000 Hazard Note Irritant Citronellol English Citronellol Usage And Synthesis Chemical Properties:

colourless liquid with a characteristic, rose-like, smell Citronellol Preparation

ProductsGeraniol-->Citronellal-->CITRONELLIC ACID-->Rose

Oil-->3,7-DIMETHYL-7-OCTEN-1-OL-->Citronellyl acetate-->CITRONELLYL

ISOBUTYRATE-->3,7-DIMETHYL-1-OCTANOL Raw

materialsEtanol-->Hydrogen-->tert-Butanol-->Ferrous sulfate

heptahydrate-->Citral-->Geraniol-->Citronellal-->NEROL-->ALPHA-PINENE-->Diisobutylalumi-

um hydride-->Eucalyptus oil-->Citronella oil-->Triisobutylaluminium-->Platinum

balck-->Dihydromyrcene-->Citronellol