



Formula: C<sub>20</sub>H<sub>40</sub>O

MW: 296.54

CAS: 505-32-8

MDL: MFCD00048380

TNP: TNP00394

1-Hexadecen-3-ol, 3,7,11,15-tetramethyl-; 1-Hexadecen-3-ol,3,7,11,15-tetramethyl-;  
1-Hexadecene-3-ol, 3,7,11,15-tetramethyl; 2,6,10,14-tetramethylhexadec-15-en-14-ol;  
2,6,10-trimethyl-14-vinylpentadecan-14-ol; 3,7,11,15-tetramethyl-1-hexadecen-3-ol;  
Hexadec-1-en



LogP: 2.49

LogS: -4.17

Acceptors: 1

Donors: 1

Rotation Bonds: 14

Chiral Centers: 3

N+O: 1

LIPINSKY: 4

Oil: LIQUID

Info: Isophytol 95%

IUPAC: 3,7,11,15-tetramethylhexadec-1-en-3-ol

Smiles: C(CCC(CCCC(CCCC(C)C)C)C)C(C=C)(C)O

Specification: Biochemistry; Terpenes; Terpenes (Others); Cnbio Isophytol Chemical Properties:

bp 309 C(lit.) density 0.841 g/mL at 25 C(lit.) refractive index n<sub>20</sub>/D 1.457(lit.) Fp >230 F Water Solubility Practically insoluble Merck 14,5198 BRN 1783243 Stability:Stable. Incompatible with strong oxidizing agents. CAS DataBase Reference505-32-8(CAS DataBase Reference) NIST Chemistry ReferenceIsophytol(505-32-8) EPA Substance Registry System1-Hexadecen-3-ol, 3,7,11,15-tetramethyl-(505-32-8) Safety Information Hazard Codes Xi Risk Statements 36/37/38 Safety Statements 24/25-37/39-26 WGK Germany 1 F 10 Hazardous Substances Data505-32-8(Hazardous Substances Data) 3,7,11,15-Tetramethyl-1-hexadecen-3-ol English Isophytol Usage And Synthesis Chemical Properties:

colourless viscous liquid Isophytol Raw materialsTetrahydrofuran-->Citral-->Methyl acetoacetate-->Linalool-->Propargyl alcohol Preparation ProductsTocopheryl acetate-->Vitamin E-->Vitamin E

Merck 13 Reference: Monograph Number: 0005217

Title: Isophytol

CAS Registry Number: 505-32-8

CAS Name: 3,7,11,15-Tetramethyl-1-hexadecen-3-ol

Additional Names: 2,6,10,14-tetramethylhexadec-15-en-14-ol;  
2,6,10-trimethyl-14-vinylpentadecan-14-ol

Molecular Formula: C<sub>20</sub>H<sub>40</sub>O

Molecular Weight: 296.53.

Percent Composition: C 81.01%, H 13.60%, O 5.40%

Literature References: Decompn product of chlorophyll. Synthesis from linalool or citral: Fischer, L