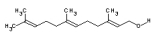

Formula: C15H26O

MW: 222.37

CAS: 4602-84-0

MDL: MFCD00002918

TNP: TNP00555

10-dodecatrien-1-ol,3,7,11-trimethyl-6; 2,6,10-trimethyl-2,6,10-dodecatrien-12-ol[qr]; 3,7,11-trimethyl-2,6,10-dodecatrien-1-ol[qr]; 3,7,11-Trimethyl-2,6,10-dodecatrienol; 6,10-Dodecatrien-1-ol,3,7,11-trimethyl-2; farnesol,mixtureofisomers; Farnesyl alcohol; far

LogP: 5.58

LogS: -4.78

Acceptors: 1

Donors: 1

Rotation Bonds: 8

Chiral Centers: 0

N+O: 1

LIPINSKY: 4

Oil: Liquid

Info: Farnesol, mixture of isomers 96% Use in perfumery

IUPAC: (2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-ol

Smiles: C(=CCCC(=CCO)C)(/CCC=C(C)C)C

Specification: Biochemistry; Terpenes; Terpenes (Others) FARNESOL Chemical Properties:

 bp 149 C4 mm Hg(lit.) density 0.886 g/mL at 20 C(lit.) refractive index n20/D 1.490(lit.) FEMA 2478 Fp 205 F storage temp. -20C Merck 14,3937 BRN 1763926 Stability:Stable. Combustible. Incompatible with strong oxidizing agents. CAS DataBase Reference4602-84-0(CAS DataBase Reference) NIST Chemistry Reference2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-(4602-84-0) EPA Substance Registry System2,6,10-Dodecatrien- 1-ol, 3,7,11-trimethyl-(4602-84-0) Safety Information Hazard Codes Xi Safety Statements 24/25-22 WGK Germany 3 RTECS JR4979000 F 8 Hazard Note Irritant Hazardous Substances Data4602-84-0(Hazardous Substances Data) FARNESOL Usage And Synthesis Chemical Properties:

colourless liquid with a floral odour General DescriptionColorless liquid with a delicate floral odor. Reactivity ProfileFlammable and/or toxic gases are generated by the combination of alcohols with alkali metals, nitrides, and strong reducing agents. They react with oxoacids and carboxylic acids to form esters plus water. Oxidizing agents convert them to aldehydes or ketones. Alcohols exhibit both weak acid and weak base behavior. They may initiate the polymerization of isocyanates and epoxides. FARNESOL Raw materialsAcetic anhydride-->Nerolidol

Merck 13 Reference: Monograph Number: 0003968

Title: Farnesol

CAS Registry Number: 4602-84-0

CAS Name: 3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol

Molecular Formula: C15H26O

Molecular Weight: 222.37.

Percent Composition: C 81.02%, H 11.79%, O 7.19%

Literature References: Found in oils of citronella, neroli, cyclamen, lemon grass, tuberose, rose, musk, balsam Peru, and tolu. Isoln: Elge, Chem. Ztg. 34, 857 (1910); 37, 1422 (1913); Kerschbaum, Ber. 46, 1732 (1913); Naves, Helv. Chim. Acta 32, 1798, 2181 (1949); LaFace, ibid. 33, 249 (1950). Synthesis: Ruzicka, ibid. 6, 492 (1923); Ruzicka, Firmenich, ibid. 22, 392 (1939); Nazarov et al., Zh. Obshch. Khim. 28, 1444 (1958); Shvarts, Petrov, ibid. 30, 3598 (1960); Popjak et al., J. Biol. Chem. 237, 56 (1962). Four possible stereoisomers. Stereochemistry: Bates et al., Chem. Ind. (London) 1961, 1907; J. Org. Chem. 28, 1086 (1963). trans-trans-Farnesol is the only stereoisomer present in many essential oils but occurs mixed with cis-trans-farnesol in petitgrain oil and several other oils: Naves, Compt. Rend. 251, 900 (1960). Stereospecific synthesis of trans-trans-farnesol: Corey et al., J. Am. Chem. Soc. 92, 6637 (1970).

Derivative Type: trans-trans-Farnesol

Properties: Liquid. bp0.35 111. nD25 1.4872. uv max: 192-196 nm (e 28,500).

Boiling point: bp0.35 111

Index of refraction: nD25 1.4872

Absorption maximum: uv max: 192-196 nm (e 28,500)

Derivative Type: Commercial farnesol

Properties: bp0.2 110-113. d420 0.8871. nD20 1.4870.

Boiling point: bp0.2 110-113

Index of refraction: nD20 1.4870

Density: d420 0.8871

Use: In perfumery, to emphasize the odor of sweet floral perfumes, such as lilac and cyclamen.