



Formula: C<sub>33</sub>H<sub>54</sub>O<sub>5</sub>

MW: 530.79

CAS: 4345-03-3

TNP NUMBER: TNP00621

MDL NUMBER: MFCD00198020

IUPAC: 3-[[[(2R)-2-((4R,8R)-4,8,12-trimethyltridecyl)-2,5,7,8-tetramethylchroman-6-yl]oxycarbonyl]propanoic acid

Smiles:

Cc1c2c(c(c(c1C)OC(CCC(=O)O)=O)C)CC[C](O2)(CCC[C@@H](CCC[C@@H](CCCC(C)C)C)C)C

Vitamin E found largely in plant materials

THERAPEUTIC CATEGORY: Antioxidants and Cytoprotectants, VITAMIN E

ACCEPTORS: 5

DONORS: 1

ROTATION BONDS: 18

N+O: 5

Chiral Centers: 3

LogP: 12.27

LogS: -8.23

LIPINSKI: 2

Synonyms:

(+)-nyl)este;(2r-(2r\*(4r\*,8r\*)))-cyl)-2h-1-benzopyran-6-yl)este;[2theta-[2theta(4theta,8theta)]]-cyl)-2h-1-benzopyran-6-yl]este;alpha-tocopherol,succinate;alpha-tocopherolhemisuccinate;butanedioicacid,mono(3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl);butanedioicacid,mono[3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl);mono[3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-yl]ester,[2R-Butanedioicacid

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EINECS:224-403-8

Product Categories:Vitamins and derivatives;Vitamin Ingredients Vitamin E succinate

Chemical Properties: mp ~76 C(lit.) storage temp. 2-8C Merck 13,9571

CAS DataBase Reference: 4345-03-3(

CAS DataBase Reference: ) EPA Substance Registry SystemButanedioic acid, mono[(2R)-3,4-dihydro-2,5, 7,8-tetramethyl-2-[(4R,8R)- 4,8,12-trimethyltridecyl]-2H-1-benzopyran-6-yl] ester(4345-03-3)

Safety Information: WGK Germany 1 RTECS EJ9984000 F 8-10-23 D-alpha-Tocopherol succinate Vitamin E succinate

Usage And Synthesis: General DescriptionWhite powder. Air & Water ReactionsInsoluble in water. Reactivity ProfileVitamin E succinate is an ester. Esters react with acids to liberate heat along with alcohols and acids. Strong oxidizing acids may cause a vigorous reaction that is sufficiently exothermic to ignite the reaction products. Heat is also generated by the interaction of esters with caustic solutions. Flammable hydrogen is generated by mixing esters with alkali metals and hydrides. Fire HazardFlash point data for Vitamin E succinate are not available; however, Vitamin E succinate is probably combustible. Vitamin E succinate

