

Vitamin E

Other names:

(+)-.alpha.-tocopherol
(+)-«alpha»-Tocopherol
(2R)-3,4-Dihydro-2,5,7,8-tetramethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-2H-1-benzopyran-6-ol
(2R,4'R,8'R)-.alpha.-tocopherol
(2R,4'R,8'R)-«alpha»-Tocopherol
(All-R)-«alpha»-Tocopherol
(R,R,R)-.alpha.-tocopherol
(R,R,R)-«alpha»-Tocopherol
(all-R)-.alpha.-tocopherol
,8,12-trimethyltridecyl)-, [2R-[2R*(4R*,8R*)]]-
.alpha.-tocopherol
121854-78-2
18920-62-2
2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-6-chromanol
2H-1-Benzopyran-6-ol,
3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2R-[2R*(4R*,8R*)]]-
3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol,
[2R-[2R*(4R*,8R*)]]-
564-49-8
5,7,8-trimethyltolcol
Almefrol
Antisterility vitamin
Aquasol E
Covi-ox
Covitol F 1000
Covitol F 1300
D-.alpha.-tocopherol
D-«alpha»-tocopherol
Denamone
E-Oil 1000
E-toplex
E-vimin
Emipherol
Endo E
Eprolin
Eprolin S
Epsilon
Epsilon-m
Esorb
Etamican
Etavit
Evion

Evipherol
 Evitaminum
 Ilitia
 Lan-E
 Med-E
 Phytogermine
 Profecundin
 Rhenogran Ronotec 50
 Spavit
 Spavit E
 Syntopherol
 Tenox GT 1
 Tocopherex
 Tocopherol
 Tokopharm
 Vascuals
 Verrol
 Vi-E
 Viprimol
 Vita E
 Vitayonon
 Viteolin
 [2R-2R*(4R*,8R*)]-3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benz
 vitamin E.alpha.
 vitaplex E
 «alpha»-D-Tocopherol
 «alpha»-Tocopherol
 «alpha»-Tokoferol
 «alpha»-Vitamin E

Inchi: InChI=1S/C29H50O2/c1-20(2)12-9-13-21(3)14-10-15-22(4)16-11-18-29(8)19-17-26-25(7)

InchiKey: GVJHHUAWPYXKBD-UHFFFAOYSA-N

Formula: C29H50O2

SMILES: Cc1c(C)c2c(c(C)c1O)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2

Mol. weight [g/mol]: 430.71

CAS: 59-02-9

Physical Properties

Property code	Value	Unit	Source
gf	62.29	kJ/mol	Joback Method

hf	-694.51		kJ/mol	Joback Method
hfus	56.28		kJ/mol	Joback Method
hvap	100.37		kJ/mol	Joback Method
log10ws	-9.77			Crippen Method
logp	8.840			Crippen Method
mcvol	396.590		ml/mol	McGowan Method
pc	882.09		kPa	Joback Method
rinpol	3149.40			NIST Webbook
rinpol	3142.00			NIST Webbook
rinpol	3112.00			NIST Webbook
rinpol	3138.00			NIST Webbook
rinpol	3149.40			NIST Webbook
rinpol	3112.00			NIST Webbook
rinpol	3130.00			NIST Webbook
rinpol	3142.00			NIST Webbook
rinpol	3138.00			NIST Webbook
tb	1027.02		K	Joback Method
tc	1257.43		K	Joback Method
tf	624.70		K	Joback Method
vc	1.468		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1437.29	J/mol×K	1027.02	Joback Method
cpg	1465.97	J/mol×K	1065.42	Joback Method
cpg	1495.02	J/mol×K	1103.82	Joback Method
cpg	1524.68	J/mol×K	1142.22	Joback Method
cpg	1555.22	J/mol×K	1180.63	Joback Method
cpg	1586.87	J/mol×K	1219.03	Joback Method
cpg	1619.91	J/mol×K	1257.43	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
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tbp

549.26

K

1.10

Boiling Points of
Short-Chain
Partial
Acylglycerols and
Tocopherols at
Low Pressures
by the Differential
Scanning
Calorimetry
Technique

Sources

Boiling Points of Short-Chain Partial
Acylglycerols and Tocopherols at Low
Pressures by the Differential Scanning
Calorimetry Technique:
Joback Method:

<https://www.doi.org/10.1021/je401080p>

McGowan Method:

<https://www.doi.org/10.1021/je7005538>

https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C59029&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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