

«delta»-Tocopherol

Other names:	(R)-2,8-Dimethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman-6-ol .omega.-tocopherol 2,8-Dimethyl-2-(4,8,12-trimethyltridecyl)-6-chromanol 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,8-dimethyl-2-(4,8,12-trimethyltridecyl)-, [2R-[2R*(4R*,8R*)]]- 2H-1-benzopyran-6-ol, 3,4-dihydro-2,8-dimethyl-2-(4,8,12-trimethyltridecyl)- 3,4-Dihydro-2,8-dimethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol 6-chromanol, 2,8-dimethyl-2-(4,8,12-trimethyltridecyl)- 8-Methyltocol [2R[2R*(4R*,8R*)]]-3,4-dihydro-2,8-dimethyl-2-(4,8,12-trimethyltridecyl)-2H-benzopyran-6-ol
Inchi:	InChI=1S/C27H46O2/c1-20(2)10-7-11-21(3)12-8-13-22(4)14-9-16-27(6)17-15-24-19-25(2)26
InchiKey:	GZIFEOYASATJEH-UHFFFAOYSA-N
Formula:	C27H46O2
SMILES:	Cc1cc(O)cc2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]:	402.65
CAS:	119-13-1

Physical Properties

Property code	Value	Unit	Source
gf	64.71	kJ/mol	Joback Method
hf	-630.29	kJ/mol	Joback Method
hfus	51.88	kJ/mol	Joback Method
hvap	94.59	kJ/mol	Joback Method
log10ws	-8.82		Crippen Method
logp	8.223		Crippen Method
mcvol	368.410	ml/mol	McGowan Method
pc	1011.02	kPa	Joback Method
rinpol	2968.10		NIST Webbook
rinpol	2951.00		NIST Webbook
rinpol	2951.00		NIST Webbook
tb	971.30	K	Joback Method
tc	1192.37	K	Joback Method
tf	577.12	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1299.97	J/mol×K	971.30	Joback Method
cpg	1325.79	J/mol×K	1008.14	Joback Method
cpg	1351.73	J/mol×K	1044.99	Joback Method
cpg	1378.03	J/mol×K	1081.83	Joback Method
cpg	1404.92	J/mol×K	1118.68	Joback Method
cpg	1432.64	J/mol×K	1155.52	Joback Method
cpg	1461.41	J/mol×K	1192.37	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	552.60	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:
McGowan Method:

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

NIST Webbook:

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

Crippen Method:

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

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C119131&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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