«beta»-Tocopherol

Other names:	2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)- 6-Chromanol, 2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)- «beta»-Tokoferol p-Xylotocopherol Cumotocopherol Neotocopherol 5,8-Dimethyltocol 3,4-Dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol 2,5,8-Trimethyl-2-(4,8,12-trimethyltridecyl)-6-chromanol 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,8-trimethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)-, (2R)-rel- 16662-70-7 3,4-dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)-2H-benzopyran-6-ol
Inchi:	InChI=1S/C28H48O2/c1-20(2)11-8-12-21(3)13-9-14-22(4)15-10-17-28(7)18-16-25-24(6)2
InchiKey:	WGVKWNUPNGFDFJ-UHFFFAOYSA-N
Formula:	C28H48O2
SMILES:	Cc1cc(O)c(C)c2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]:	416.68
CAS:	148-03-8

Physical Properties

Property code	Value	Unit	Source
gf	63.50	kJ/mol	Joback Method
hf	-662.40	kJ/mol	Joback Method
hfus	54.08	kJ/mol	Joback Method
hvap	97.48	kJ/mol	Joback Method
log10ws	-9.29		Crippen Method
logp	8.532		Crippen Method
mcvol	382.500	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	3076.00		NIST Webbook
rinpol	3043.00		NIST Webbook
tb	999.16	K	Joback Method
tc	1224.33	K	Joback Method
tf	600.91	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1368.02	J/mol×K	999.16	Joback Method
cpg	1395.17	J/mol×K	1036.69	Joback Method
cpg	1422.57	J/mol×K	1074.22	Joback Method
cpg	1450.44	J/mol×K	1111.74	Joback Method
cpg	1479.04	J/mol×K	1149.27	Joback Method
cpg	1508.61	J/mol×K	1186.80	Joback Method
cpg	1539.38	J/mol×K	1224.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C148038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/60-239-0/beta-Tocopherol.pdf

Generated by Cheméo on 2024-05-01 22:02:50.258139331 +0000 UTC m=+16890219.178716647.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.