Tocotrienol, 5,8-dimethyl

Inchi: InChI=1S/C28H42O2/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: FGYKUFVNYVMTAM-UXRPBPJUSA-N
Formula: C28H42O2
SMILES: CC(C)=CCCC(C)=CCCC(C)=CCCC1(C)CCc2c(C)c(O)cc(C)c2O1
Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	285.83	kJ/mol	Joback Method
hf	-324.27	kJ/mol	Joback Method
hfus	61.32	kJ/mol	Joback Method
hvap	98.76	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	8.292		Crippen Method
mcvol	369.600	ml/mol	McGowan Method
pc	1034.57	kPa	Joback Method
rinpol	3069.00		NIST Webbook
tb	1012.60	K	Joback Method
tc	1244.99	K	Joback Method
tf	588.79	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.49	J/mol×K	1012.60	Joback Method
cpg	1311.78	J/mol×K	1051.33	Joback Method
cpg	1341.08	J/mol×K	1090.06	Joback Method
cpg	1371.73	J/mol×K	1128.80	Joback Method
cpg	1404.03	J/mol×K	1167.53	Joback Method
cpg	1438.31	J/mol×K	1206.26	Joback Method
cpg	1474.89	J/mol×K	1244.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R523029&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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