

Tocotrienol, 5-methyl

Inchi:	InChI=1S/C27H40O2/c1-20(2)10-7-11-21(3)12-8-13-22(4)14-9-18-27(6)19-17-24-23(5)25
InchiKey:	NWELWDHWNAURGA-NDZYPVAJSA-N
Formula:	C27H40O2
SMILES:	CC(C)=CCCC(C)=CCCC(C)=CCCC1(C)CCc2c(ccc(O)c2C)O1
Mol. weight [g/mol]:	396.61

Physical Properties

Property code	Value	Unit	Source
gf	287.04	kJ/mol	Joback Method
hf	-292.16	kJ/mol	Joback Method
hfus	59.12	kJ/mol	Joback Method
hvap	95.87	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	7.984		Crippen Method
mcvol	355.510	ml/mol	McGowan Method
pc	1112.59	kPa	Joback Method
rinsol	3060.00		NIST Webbook
tb	984.74	K	Joback Method
tc	1214.90	K	Joback Method
tf	565.00	K	Joback Method
vc	1.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.39	J/mol×K	984.74	Joback Method
cpg	1242.04	J/mol×K	1023.10	Joback Method
cpg	1269.54	J/mol×K	1061.46	Joback Method
cpg	1298.21	J/mol×K	1099.82	Joback Method
cpg	1328.37	J/mol×K	1138.18	Joback Method
cpg	1360.32	J/mol×K	1176.54	Joback Method
cpg	1394.38	J/mol×K	1214.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R523034&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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