Tocotrienol

Inchi: InChI=1S/C26H38O2/c1-20(2)9-6-10-21(3)11-7-12-22(4)13-8-17-26(5)18-16-23-19-24(27
InchiKey: GJJVAFUKOBZPCB-CEPFXNDVSA-N
Formula: C26H38O2
SMILES: CC(C)=CCCC(C)=CCCC(C)=CCCC1(C)CCc2cc(O)ccc2O1
Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	288.25	kJ/mol	Joback Method
hf	-260.05	kJ/mol	Joback Method
hfus	56.92	kJ/mol	Joback Method
hvap	92.98	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	7.675		Crippen Method
mcvol	341.420	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinpol	2963.00		NIST Webbook
rinpol	2963.00		NIST Webbook
tb	956.88	K	Joback Method
tc	1185.80	K	Joback Method
tf	541.21	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.83	J/mol×K	956.88	Joback Method
cpg	1174.03	J/mol×K	995.03	Joback Method
cpg	1199.93	J/mol×K	1033.19	Joback Method
cpg	1226.84	J/mol×K	1071.34	Joback Method
cpg	1255.06	J/mol×K	1109.50	Joback Method
cpg	1284.92	J/mol×K	1147.65	Joback Method
cpg	1316.73	J/mol×K	1185.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522997&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