«delta»-Tocopherol, O-methyl-

Inchi: InChI=1S/C28H48O2/c1-21(2)11-8-12-22(3)13-9-14-23(4)15-10-17-28(6)18-16-25-20-26
InchiKey: NWSJWTQKDPRHML-UHFFFAOYSA-N
Formula: C28H48O2
SMILES: COc1cc(C)c2c(c1)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2
Mol. weight [g/mol]: 416.68

Physical Properties

Property code	Value	Unit	Source
gf	113.12	kJ/mol	Joback Method
hf	-617.31	kJ/mol	Joback Method
hfus	49.48	kJ/mol	Joback Method
hvap	86.87	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	8.526		Crippen Method
mcvol	382.500	ml/mol	McGowan Method
pc	853.96	kPa	Joback Method
rinpol	2887.00		NIST Webbook
rinpol	2887.00		NIST Webbook
tb	940.96	K	Joback Method
tc	1154.27	K	Joback Method
tf	511.42	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1324.02	J/mol×K	940.96	Joback Method
cpg	1348.72	J/mol×K	976.51	Joback Method
cpg	1372.83	J/mol×K	1012.06	Joback Method
cpg	1396.50	J/mol×K	1047.62	Joback Method
cpg	1419.89	J/mol×K	1083.17	Joback Method
cpg	1443.14	J/mol×K	1118.72	Joback Method
cpg	1466.42	J/mol×K	1154.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374728&Units=SI

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