Tocol

Inchi: InChI=1S/C26H44O2/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: DFUSDJMZWQVQSF-MCEYFSPLSA-N
Formula: C26H44O2
SMILES: CC(C)CCCC(C)CCCC(C)CCCC1(C)CCc2cc(O)ccc2O1
Mol. weight [g/mol]: 388.63

Physical Properties

Property code	Value	Unit	Source
gf	65.92	kJ/mol	Joback Method
hf	-598.18	kJ/mol	Joback Method
hfus	49.68	kJ/mol	Joback Method
hvap	91.70	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	7.915		Crippen Method
mcvol	354.320	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	2867.00		NIST Webbook
tb	943.44	K	Joback Method
tc	1161.46	K	Joback Method
tf	553.33	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1233.16	J/mol×K	943.44	Joback Method
cpg	1257.82	J/mol×K	979.78	Joback Method
cpg	1282.48	J/mol×K	1016.11	Joback Method
cpg	1307.40	J/mol×K	1052.45	Joback Method
cpg	1332.78	J/mol×K	1088.78	Joback Method
cpg	1358.86	J/mol×K	1125.12	Joback Method
cpg	1385.87	J/mol×K	1161.46	Joback Method

Sources

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=R522917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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