Tocol, 8-methyl

Inchi: InChI=1S/C27H46O2/c1-20(2)10-7-11-21(3)12-8-13-22(4)14-9-16-27(6)17-15-24-19-25(2
InchiKey: GZIFEOYASATJEH-BERHBOFZSA-N
Formula: C27H46O2
SMILES: Cc1cc(O)cc2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]: 402.65

Physical Properties

Property code	Value	Unit	Source
gf	64.71	kJ/mol	Joback Method
hf	-630.29	kJ/mol	Joback Method
hfus	51.88	kJ/mol	Joback Method
hvap	94.59	kJ/mol	Joback Method
log10ws	-8.82		Crippen Method
logp	8.223		Crippen Method
mcvol	368.410	ml/mol	McGowan Method
pc	1011.02	kPa	Joback Method
rinpol	2889.00		NIST Webbook
tb	971.30	K	Joback Method
tc	1192.37	K	Joback Method
tf	577.12	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1299.97	J/mol×K	971.30	Joback Method
cpg	1325.79	J/mol×K	1008.14	Joback Method
cpg	1351.73	J/mol×K	1044.99	Joback Method
cpg	1378.03	J/mol×K	1081.83	Joback Method
cpg	1404.92	J/mol×K	1118.68	Joback Method
cpg	1432.64	J/mol×K	1155.52	Joback Method
cpg	1461.41	J/mol×K	1192.37	Joback Method

Sources

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=R522982&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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