Tocol, 7,8-dimethyl

Inchi: InChI=1S/C28H48O2/c1-20(2)11-8-12-21(3)13-9-14-22(4)15-10-17-28(7)18-16-25-19-26
InchiKey: QUEDXNHFTDJVIY-VPYPWEPUSA-N
Formula: C28H48O2
SMILES: Cc1c(O)cc2c(c1C)OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]: 416.68

Physical Properties

Property code	Value	Unit	Source
gf	63.50	kJ/mol	Joback Method
hf	-662.40	kJ/mol	Joback Method
hfus	54.08	kJ/mol	Joback Method
hvap	97.48	kJ/mol	Joback Method
log10ws	-9.29		Crippen Method
logp	8.532		Crippen Method
mcvol	382.500	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	2987.00		NIST Webbook
rinpol	2987.00		NIST Webbook
tb	999.16	K	Joback Method
tc	1224.33	K	Joback Method
tf	600.91	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1368.02	J/mol×K	999.16	Joback Method
cpg	1395.17	J/mol×K	1036.69	Joback Method
cpg	1422.57	J/mol×K	1074.22	Joback Method
cpg	1450.44	J/mol×K	1111.74	Joback Method
cpg	1479.04	J/mol×K	1149.27	Joback Method
cpg	1508.61	J/mol×K	1186.80	Joback Method
cpg	1539.38	J/mol×K	1224.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522962&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

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