Prenopsan-8-ol

Inchi: InChI=1S/C15H28O/c1-12-6-5-7-14(4)8-9-15(12,16)11-13(2,3)10-14/h12,16H,5-11H2,1-4
InchiKey: OUUHVBGIOSOUTO-DJIKBVBFSA-N
Formula: C15H28O
SMILES: CC1CCCC2(C)CCC1(O)CC(C)(C)C2
Mol. weight [g/mol]: 224.38

Physical Properties

Property code	Value	Unit	Source
gf	-32.29	kJ/mol	Joback Method
hf	-385.32	kJ/mol	Joback Method
hfus	7.71	kJ/mol	Joback Method
hvap	62.28	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.144		Crippen Method
mcvol	206.360	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1574.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	660.99	K	Joback Method
tc	880.55	K	Joback Method
tf	401.13	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.95	J/mol×K	660.99	Joback Method
cpg	637.59	J/mol×K	697.58	Joback Method
cpg	658.45	J/mol×K	734.18	Joback Method
cpg	678.85	J/mol×K	770.77	Joback Method
cpg	699.09	J/mol×K	807.36	Joback Method

cpg	719.48	J/mol×K	843.96	Joback Method
cpg	740.34	J/mol×K	880.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R513676&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

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