13R,S-14,15-Dinorlabdane-8,13-diol

Inchi: InChI=1S/C18H34O2/c1-13(19)7-8-15-17(4)11-6-10-16(2,3)14(17)9-12-18(15,5)20/h13-1
InchiKey: HFEFNSOKHKUOER-VKLUZWIXSA-N
Formula: C18H34O2
SMILES: CC(O)CCC1C(C)(O)CCC2C(C)(C)CCCC21C
Mol. weight [g/mol]: 282.46

Physical Properties

Property code	Value	Unit	Source
gf	-141.90	kJ/mol	Joback Method
hf	-618.93	kJ/mol	Joback Method
hfus	19.22	kJ/mol	Joback Method
hvap	84.77	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.141		Crippen Method
mcvol	254.500	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	812.43	K	Joback Method
tc	1013.29	K	Joback Method
tf	480.04	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.16	J/mol×K	812.43	Joback Method
cpg	886.96	J/mol×K	845.91	Joback Method
cpg	909.01	J/mol×K	879.38	Joback Method
cpg	931.56	J/mol×K	912.86	Joback Method
cpg	954.86	J/mol×K	946.34	Joback Method
cpg	979.16	J/mol×K	979.81	Joback Method
cpg	1004.71	J/mol×K	1013.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R290412&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