6,9-Dihydroxyhumulenol

Inchi: InChI=1S/C15H28O2/c1-11-5-6-14(17)12(2)9-13(16)10-15(3,4)8-7-11/h7,12-14,16-17H,5
InchiKey: LLPBXVXTTBILMJ-YRNVUSSQSA-N
Formula: C15H28O2
SMILES: CC1=CCC(C)(C)CC(O)CC(C)C(O)CC1
Mol. weight [g/mol]: 240.38

Physical Properties

Property code	Value	Unit	Source
gf	-242.56	kJ/mol	Joback Method
hf	-633.34	kJ/mol	Joback Method
hfus	21.86	kJ/mol	Joback Method
hvap	82.51	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.281		Crippen Method
mcvol	218.790	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1822.00		NIST Webbook
rinpol	1822.00		NIST Webbook
tb	758.23	K	Joback Method
tc	960.13	K	Joback Method
tf	394.69	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.27	J/mol×K	758.23	Joback Method
cpg	718.37	J/mol×K	791.88	Joback Method
cpg	736.51	J/mol×K	825.53	Joback Method
cpg	753.76	J/mol×K	859.18	Joback Method
cpg	770.17	J/mol×K	892.83	Joback Method
cpg	785.80	J/mol×K	926.48	Joback Method
cpg	800.69	J/mol×K	960.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R628778&Units=SI

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