Humuladienol

Inchi: InChI=1S/C15H26O/c1-12-7-8-14(16)13(2)6-5-10-15(3,4)11-9-12/h5,9-10,13-14,16H,6-8
InchiKey: JXLVPCWSMFUWOE-VKLURXMVSA-N
Formula: C15H26O
SMILES: CC1=CCC(C)(C)C=CCC(C)C(O)CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	-68.07	kJ/mol	Joback Method
hf	-402.99	kJ/mol	Joback Method
hfus	17.93	kJ/mol	Joback Method
hvap	66.43	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.086		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1546.00		NIST Webbook
rinpol	1546.00		NIST Webbook
tb	669.88	K	Joback Method
tc	884.88	K	Joback Method
tf	338.87	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.52	J/mol×K	669.88	Joback Method
cpg	621.01	J/mol×K	705.71	Joback Method
cpg	641.36	J/mol×K	741.55	Joback Method
cpg	660.64	J/mol×K	777.38	Joback Method
cpg	678.92	J/mol×K	813.22	Joback Method
cpg	696.28	J/mol×K	849.05	Joback Method
cpg	712.77	J/mol×K	884.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225448&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