humulenol II

Inchi: InChI=1S/C15H24O/c1-12-7-5-9-13(2)14(16)11-15(3,4)10-6-8-12/h6-7,10,14,16H,2,5,8-9
InchiKey: NMGJCQNNUTYSJJ-KCYZJYRFSA-N
Formula: C15H24O
SMILES: C=C1CCC=C(C)CC=CC(C)(C)CC1O
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	-7.28	kJ/mol	Joback Method
hf	-298.41	kJ/mol	Joback Method
hfus	15.70	kJ/mol	Joback Method
hvap	66.90	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.006		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2285.00		NIST Webbook
ripol	2314.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2274.00		NIST Webbook
ripol	2234.00		NIST Webbook
tb	673.71	K	Joback Method
tc	890.35	K	Joback Method
tf	356.79	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.42	J/mol×K	673.71	Joback Method

cpg	593.46	J/mol×K	709.82	Joback Method
cpg	612.44	J/mol×K	745.92	Joback Method
cpg	630.44	J/mol×K	782.03	Joback Method
cpg	647.51	J/mol×K	818.13	Joback Method
cpg	663.75	J/mol×K	854.24	Joback Method
cpg	679.22	J/mol×K	890.35	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=R210109&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume