Humulenol

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-WRKUNCLDSA-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
ripol	2265.00		NIST Webbook
ripol	2265.00		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

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=R569218&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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