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=C1CC/C=C(\C)C/C=C/C(C)(C)C[C@H]1O
Mol. weight [g/mol]: 220.36

Physical Properties

Property code	Value	Unit	Source
hfus	15.70	kJ/mol	Joback Method
hvap	90.54	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
logp	4.006		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2314.00		NIST Webbook
ripol	2285.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2234.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2274.00		NIST Webbook
tb	576.28	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R210109&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature