«alpha»-Humulene hydrate

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

Physical Properties

Property code	Value	Unit	Source
gf	-65.85	kJ/mol	Joback Method
hf	-367.41	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	65.59	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1597.00		NIST Webbook
rinpol	1597.00		NIST Webbook
tb	674.79	K	Joback Method
tc	897.41	K	Joback Method
tf	367.01	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.94	J/mol×K	674.79	Joback Method
cpg	615.03	J/mol×K	711.89	Joback Method
cpg	635.21	J/mol×K	749.00	Joback Method
cpg	654.65	J/mol×K	786.10	Joback Method
cpg	673.53	J/mol×K	823.20	Joback Method
cpg	692.04	J/mol×K	860.30	Joback Method
cpg	710.36	J/mol×K	897.41	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=R626123&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume