iso-«alpha»-humulene

Inchi: InChI=1S/C15H24/c1-13-7-5-8-14(2)10-12-15(3,4)11-6-9-13/h7,10,12H,2,5-6,8-9,11H2,1
InchiKey: FNXUOGPQAOCFKU-RYKBTYGJSA-N
Formula: C15H24
SMILES: C=C1C=CC(C)(C)CCCC(C)=CCC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	137.25	kJ/mol	Joback Method
hf	-125.84	kJ/mol	Joback Method
hfus	10.54	kJ/mol	Joback Method
hvap	50.53	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1471.00		NIST Webbook
tb	586.20	K	Joback Method
tc	821.65	K	Joback Method
tf	300.21	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.47	J/mol×K	586.20	Joback Method
cpg	523.64	J/mol×K	625.44	Joback Method
cpg	546.38	J/mol×K	664.68	Joback Method
cpg	567.79	J/mol×K	703.92	Joback Method
cpg	587.97	J/mol×K	743.17	Joback Method
cpg	607.03	J/mol×K	782.41	Joback Method
cpg	625.07	J/mol×K	821.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R406370&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