Dihydrohumulene

Inchi: InChI=1S/C15H26/c1-13-7-5-8-14(2)10-12-15(3,4)11-6-9-13/h6-7,11,14H,5,8-10,12H2,1-
InchiKey: KPNMFYMJBVVPSP-NBPRNCBBSA-N
Formula: C15H26
SMILES: CC1=CCCC(C)CCC(C)(C)C=CC1
Mol. weight [g/mol]: 206.37

Physical Properties

Property code	Value	Unit	Source
gf	76.46	kJ/mol	Joback Method
hf	-230.42	kJ/mol	Joback Method
hfus	12.77	kJ/mol	Joback Method
hvap	50.06	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	5.115		Crippen Method
mcvol	202.750	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1483.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1678.00		NIST Webbook
tb	582.37	K	Joback Method
tc	815.77	K	Joback Method
tf	282.29	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.32	J/mol×K	582.37	Joback Method
cpg	547.27	J/mol×K	621.27	Joback Method
cpg	571.70	J/mol×K	660.17	Joback Method
cpg	594.71	J/mol×K	699.07	Joback Method
cpg	616.40	J/mol×K	737.97	Joback Method

cpg	636.86	J/mol×K	776.87	Joback Method
cpg	656.19	J/mol×K	815.77	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=R207737&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume