cis-Sesquisabinene hydrate

Inchi: InChI=1S/C15H26O/c1-11(2)6-5-7-12(3)15-9-8-14(4,16)13(15)10-15/h6,12-13,16H,5,7-1
InchiKey: IRDFGGRWKUKANK-LOKSQKBWSA-N
Formula: C15H26O
SMILES: CC(C)=CCCC(C)C12CCC(C)(O)C1C2
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	110.64	kJ/mol	Joback Method
hf	-247.27	kJ/mol	Joback Method
hfus	18.81	kJ/mol	Joback Method
hvap	62.53	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1559.00		NIST Webbook
tb	647.67	K	Joback Method
tc	844.14	K	Joback Method
tf	365.03	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.77	J/mol×K	647.67	Joback Method
cpg	600.91	J/mol×K	680.41	Joback Method
cpg	617.33	J/mol×K	713.16	Joback Method
cpg	633.24	J/mol×K	745.90	Joback Method
cpg	648.84	J/mol×K	778.65	Joback Method
cpg	664.35	J/mol×K	811.39	Joback Method
cpg	679.97	J/mol×K	844.14	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R615495&Units=SI

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