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
hfus	18.81	kJ/mol	Joback Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan 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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58319054&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):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume