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-NEXFUWMNSA-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	1547.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1588.00		NIST Webbook
ripol	1997.00		NIST Webbook
ripol	2018.00		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=R313976&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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