«beta»-caryophyllene hydrate

Inchi: InChI=1S/C15H26O/c1-11-6-5-8-15(4,16)9-7-13-12(11)10-14(13,2)3/h12-13,16H,1,5-10H
InchiKey: KTBROVRYPKGILD-UHFFFAOYSA-N
Formula: C15H26O
SMILES: C=C1CCCC(C)(O)CCC2C1CC2(C)C
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	26.28	kJ/mol	Joback Method
hf	-316.32	kJ/mol	Joback Method
hfus	12.85	kJ/mol	Joback Method
hvap	63.59	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1553.00		NIST Webbook
rinpol	1553.00		NIST Webbook
ripol	2021.00		NIST Webbook
tb	659.91	K	Joback Method
tc	873.53	K	Joback Method
tf	390.91	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.57	J/mol×K	659.91	Joback Method
cpg	616.20	J/mol×K	695.51	Joback Method
cpg	635.93	J/mol×K	731.12	Joback Method
cpg	654.95	J/mol×K	766.72	Joback Method
cpg	673.48	J/mol×K	802.32	Joback Method
cpg	691.70	J/mol×K	837.93	Joback Method
cpg	709.81	J/mol×K	873.53	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=R238187&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