Caryophylla-3,8(15)-dien-5«beta»-ol

Inchi: InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h5,12-14,16H,1,6-9
InchiKey: DWUYGFWOANEJRE-RQCPJFOESA-N
Formula: C15H24O
SMILES: C=C1CCC(O)C(C)=CCCC(C)(C)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	-37.24	kJ/mol	Joback Method
hf	-356.19	kJ/mol	Joback Method
hfus	14.48	kJ/mol	Joback Method
hvap	66.61	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1661.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1675.00		NIST Webbook
ripol	2398.00		NIST Webbook
tb	674.55	K	Joback Method
tc	889.40	K	Joback Method
tf	356.03	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.82	J/mol×K	674.55	Joback Method
cpg	617.83	J/mol×K	710.36	Joback Method
cpg	637.75	J/mol×K	746.17	Joback Method
cpg	656.63	J/mol×K	781.97	Joback Method
cpg	674.56	J/mol×K	817.78	Joback Method

cpg	691.61	J/mol×K	853.59	Joback Method
cpg	707.83	J/mol×K	889.40	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=R227197&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