Caryophylla-3(15),7-dienol (6) II

Inchi: InChI=1S/C15H24O/c1-10-5-7-13-12(9-15(13,3)4)11(2)14(16)8-6-10/h13-14,16H,1,5-9H2
InchiKey: SITZSLWMRATRGJ-CPVPWXCSSA-N
Formula: C15H24O
SMILES: C=C1CCC(O)C(C)=C2CC(C)(C)C2CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	50.18	kJ/mol	Joback Method
hf	-276.38	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.840		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1682.00		NIST Webbook
tb	673.46	K	Joback Method
tc	883.37	K	Joback Method
tf	397.05	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.05	J/mol×K	673.46	Joback Method
cpg	592.93	J/mol×K	708.44	Joback Method
cpg	610.88	J/mol×K	743.43	Joback Method
cpg	628.04	J/mol×K	778.41	Joback Method
cpg	644.49	J/mol×K	813.40	Joback Method
cpg	660.35	J/mol×K	848.38	Joback Method
cpg	675.74	J/mol×K	883.37	Joback Method

Sources

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=R442049&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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