1,6-cis-Lippifolian-1 «alpha»-ol-5-one

Inchi: InChI=1S/C15H24O2/c1-9-5-6-15(17)12(11(9)16)13(2,3)7-10-8-14(10,15)4/h9-10,12,17H
InchiKey: ARIMXCACVHKASK-VZBCLDGYSA-N
Formula: C15H24O2
SMILES: CC1CCC2(O)C(C1=O)C(C)(C)CC1CC12C
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-65.54	kJ/mol	Joback Method
hf	-452.08	kJ/mol	Joback Method
hfus	12.73	kJ/mol	Joback Method
hvap	65.61	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.789		Crippen Method
mcvol	197.070	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
tb	718.07	K	Joback Method
tc	942.52	K	Joback Method
tf	493.61	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.75	J/mol×K	718.07	Joback Method
cpg	652.81	J/mol×K	755.48	Joback Method
cpg	672.70	J/mol×K	792.89	Joback Method
cpg	692.78	J/mol×K	830.29	Joback Method
cpg	713.39	J/mol×K	867.70	Joback Method
cpg	734.88	J/mol×K	905.11	Joback Method
cpg	757.61	J/mol×K	942.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R421166&Units=SI
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

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