Lippifoli-1(6)-en-4 «beta»-ol-5-one

Inchi: InChI=1S/C15H22O2/c1-13(2)7-9-8-14(9,3)10-5-6-15(4,17)12(16)11(10)13/h9,17H,5-8H2
InchiKey: QDNBEGKPBFOPJU-TURNYIBQSA-N
Formula: C15H22O2
SMILES: CC1(C)CC2CC2(C)C2=C1C(=O)C(C)(O)CC2
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-39.42	kJ/mol	Joback Method
hf	-376.56	kJ/mol	Joback Method
hfus	11.03	kJ/mol	Joback Method
hvap	67.85	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.853		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook
tb	736.53	K	Joback Method
tc	964.28	K	Joback Method
tf	527.89	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.18	J/mol×K	736.53	Joback Method
cpg	619.54	J/mol×K	774.49	Joback Method
cpg	638.09	J/mol×K	812.45	Joback Method
cpg	657.19	J/mol×K	850.40	Joback Method
cpg	677.23	J/mol×K	888.36	Joback Method
cpg	698.56	J/mol×K	926.32	Joback Method
cpg	721.55	J/mol×K	964.28	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=R421240&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume