Spirovetiva-3,7(11)-dien-12-ol

Inchi: InChI=1S/C14H22O2/c1-9-4-5-12(16)14(3)7-6-11(13(9)14)8-10(2)15/h11-13,16H,1,4-8H
InchiKey: RRLLRBBKPAUQCW-GNRIBBGQSA-N
Formula: C14H22O2
SMILES: C=C1CCC(O)C2(C)CCC(CC(C)=O)C12
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	-81.37	kJ/mol	Joback Method
hf	-411.18	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	68.91	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.709		Crippen Method
mcvol	189.540	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	682.12	K	Joback Method
tc	886.15	K	Joback Method
tf	412.71	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.53	J/mol×K	682.12	Joback Method
cpg	580.70	J/mol×K	716.12	Joback Method
cpg	597.05	J/mol×K	750.13	Joback Method
cpg	612.69	J/mol×K	784.13	Joback Method
cpg	627.74	J/mol×K	818.14	Joback Method
cpg	642.31	J/mol×K	852.14	Joback Method
cpg	656.51	J/mol×K	886.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R199290&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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