Isocurcumenol

Inchi: InChI=1S/C15H22O2/c1-9(2)13-8-14-11(4)5-6-12(14)10(3)7-15(13,16)17-14/h7,11-12,16
InchiKey: ISFMXVMWEWLJGJ-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CC1=CC2(O)OC3(CC2=C(C)C)C(C)CCC13
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	49.08	kJ/mol	Joback Method
hf	-308.39	kJ/mol	Joback Method
hfus	25.20	kJ/mol	Joback Method
hvap	69.47	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.177		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
ripol	2403.00		NIST Webbook
ripol	2403.00		NIST Webbook
tb	696.96	K	Joback Method
tc	912.86	K	Joback Method
tf	446.22	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.31	J/mol×K	696.96	Joback Method
cpg	598.15	J/mol×K	732.94	Joback Method
cpg	614.54	J/mol×K	768.93	Joback Method
cpg	630.74	J/mol×K	804.91	Joback Method
cpg	647.03	J/mol×K	840.89	Joback Method
cpg	663.66	J/mol×K	876.88	Joback Method
cpg	680.91	J/mol×K	912.86	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=R336959&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume