epi-ligulyl oxide

Inchi: InChI=1S/C15H26O/c1-10-5-7-12-9-15(16-14(12,3)4)11(2)6-8-13(10)15/h10-13H,5-9H2,1
InchiKey: GXMJXGUEPXEOGR-NWGXIFETSA-N
Formula: C15H26O
SMILES: CC1CCC2CC3(OC2(C)C)C(C)CCC13
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	101.14	kJ/mol	Joback Method
hf	-315.55	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	50.52	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.016		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1554.00		NIST Webbook
rinpol	1535.00		NIST Webbook
tb	589.05	K	Joback Method
tc	816.69	K	Joback Method
tf	363.72	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.58	J/mol×K	589.05	Joback Method
cpg	586.42	J/mol×K	626.99	Joback Method
cpg	609.68	J/mol×K	664.93	Joback Method
cpg	631.66	J/mol×K	702.87	Joback Method
cpg	652.64	J/mol×K	740.81	Joback Method
cpg	672.91	J/mol×K	778.75	Joback Method
cpg	692.75	J/mol×K	816.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R303885&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