1,10;7,10-Bisepoxy-1,10-seco-calamenene

Inchi: InChI=1S/C14H18O2/c1-10(2)14-9-8-13(3,16-14)15-12-7-5-4-6-11(12)14/h4-7,10H,8-9H2
InchiKey: DMGNVVXBTUCRCK-ARLHGKGLSA-N
Formula: C14H18O2
SMILES: CC(C)C12CCC(C)(Oc3ccccc31)O2
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
gf	105.62	kJ/mol	Joback Method
hf	-200.43	kJ/mol	Joback Method
hfus	21.78	kJ/mol	Joback Method
hvap	55.85	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.457		Crippen Method
mcvol	174.380	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1573.00		NIST Webbook
ripol	2049.00		NIST Webbook
tb	618.80	K	Joback Method
tc	861.89	K	Joback Method
tf	408.30	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.86	J/mol×K	618.80	Joback Method
cpg	493.45	J/mol×K	659.31	Joback Method
cpg	509.92	J/mol×K	699.83	Joback Method
cpg	525.66	J/mol×K	740.34	Joback Method
cpg	541.03	J/mol×K	780.86	Joback Method
cpg	556.40	J/mol×K	821.37	Joback Method
cpg	572.16	J/mol×K	861.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229475&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume