1,11-Calamenene oxide

Inchi: InChI=1S/C14H18O/c1-13(2)11-8-9-14(3,15-13)12-7-5-4-6-10(11)12/h4-7,11H,8-9H2,1-3
InchiKey: UPULKYWOGKVXOB-BXUZGUMPSA-N
Formula: C14H18O
SMILES: CC12CCC(c3ccccc31)C(C)(C)O2
Mol. weight [g/mol]: 202.29

Physical Properties

Property code	Value	Unit	Source
gf	186.47	kJ/mol	Joback Method
hf	-83.49	kJ/mol	Joback Method
hfus	18.39	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.588		Crippen Method
mcvol	168.510	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
tb	587.62	K	Joback Method
tc	828.85	K	Joback Method
tf	392.49	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.95	J/mol×K	587.62	Joback Method
cpg	464.65	J/mol×K	627.82	Joback Method
cpg	482.01	J/mol×K	668.03	Joback Method
cpg	498.38	J/mol×K	708.23	Joback Method
cpg	514.11	J/mol×K	748.44	Joback Method
cpg	529.56	J/mol×K	788.64	Joback Method
cpg	545.09	J/mol×K	828.85	Joback Method

Sources

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=R587350&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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