Calacorene oxide

Inchi: InChI=1S/C15H20O/c1-9(2)11-8-14-15(4,16-14)13-6-5-10(3)7-12(11)13/h5-7,9,11,14H,8
InchiKey: RLWKXCFJGCFMEM-UHFFFAOYSA-N
Formula: C15H20O
SMILES: Cc1ccc2c(c1)C(C(C)C)CC1OC21C
Mol. weight [g/mol]: 216.32

Physical Properties

Property code	Value	Unit	Source
gf	200.41	kJ/mol	Joback Method
hf	-129.96	kJ/mol	Joback Method
hfus	25.47	kJ/mol	Joback Method
hvap	54.90	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.752		Crippen Method
mcvol	182.600	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1643.00		NIST Webbook
rinpol	1643.00		NIST Webbook
tb	610.53	K	Joback Method
tc	835.78	K	Joback Method
tf	380.90	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.21	J/mol×K	610.53	Joback Method
cpg	515.78	J/mol×K	648.07	Joback Method
cpg	533.17	J/mol×K	685.61	Joback Method
cpg	549.61	J/mol×K	723.16	Joback Method
cpg	565.27	J/mol×K	760.70	Joback Method
cpg	580.38	J/mol×K	798.24	Joback Method
cpg	595.12	J/mol×K	835.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R78755&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