Zerumbone epoxide

Inchi: InChI=1S/C15H22O2/c1-11-6-5-8-15(4)13(17-15)10-14(2,3)9-7-12(11)16/h6-7,9,13H,5,8
InchiKey: UXYYOHOTPOQJPD-MHLOZHTBSA-N
Formula: C15H22O2
SMILES: CC1=CCCC2(C)OC2CC(C)(C)C=CC1=O
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-52.79	kJ/mol	Joback Method
hf	-399.76	kJ/mol	Joback Method
hfus	16.29	kJ/mol	Joback Method
hvap	57.23	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.426		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	675.58	K	Joback Method
tc	928.30	K	Joback Method
tf	425.96	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.32	J/mol×K	675.58	Joback Method
cpg	598.92	J/mol×K	717.70	Joback Method
cpg	620.51	J/mol×K	759.82	Joback Method
cpg	641.35	J/mol×K	801.94	Joback Method
cpg	661.72	J/mol×K	844.06	Joback Method
cpg	681.91	J/mol×K	886.18	Joback Method
cpg	702.18	J/mol×K	928.30	Joback Method

Sources

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=R121896&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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