6,7-Epoxy himachalene

Other names: Himachalen oxide («beta»)
(+)-«beta»-Himachalene oxide
Inchi: InChI=1S/C15H24O/c1-11-6-9-15-12(10-11)13(2,3)7-5-8-14(15,4)16-15/h10,12H,5-9H2,1
InchiKey: FDCRKPAGAMPEAD-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1=CC2C(C)(C)CCCC3(C)OC23CC1
Mol. weight [g/mol]: 220.35
CAS: 57819-73-5

Physical Properties

Property code	Value	Unit	Source
gf	131.40	kJ/mol	Joback Method
hf	-213.32	kJ/mol	Joback Method
hfus	13.70	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.080		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1619.00		NIST Webbook
ripol	2004.00		NIST Webbook
ripol	2045.00		NIST Webbook
tb	602.77	K	Joback Method
tc	842.98	K	Joback Method
tf	409.38	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.54	J/mol×K	602.77	Joback Method
cpg	559.70	J/mol×K	642.81	Joback Method
cpg	580.49	J/mol×K	682.84	Joback Method

cpg	600.39	J/mol×K	722.88	Joback Method
cpg	619.85	J/mol×K	762.91	Joback Method
cpg	639.36	J/mol×K	802.95	Joback Method
cpg	659.36	J/mol×K	842.98	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=C57819735&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume