2,5-epoxy-megastigma-6(Z),8(E)-diene

Inchi: InChI=1S/C13H20O/c1-5-6-7-10-12(2,3)11-8-9-13(10,4)14-11/h5-7,11H,8-9H2,1-4H3/b6-
InchiKey: RRUCICKXWFEVIP-WEYXYWBQSA-N
Formula: C13H20O
SMILES: CC=CC=C1C2(C)CCC(O2)C1(C)C
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	188.85	kJ/mol	Joback Method
hf	-100.82	kJ/mol	Joback Method
hfus	20.57	kJ/mol	Joback Method
hvap	47.17	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.466		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1312.00		NIST Webbook
tb	548.15	K	Joback Method
tc	769.15	K	Joback Method
tf	344.04	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.03	J/mol×K	548.15	Joback Method
cpg	448.63	J/mol×K	584.98	Joback Method
cpg	465.85	J/mol×K	621.82	Joback Method
cpg	481.96	J/mol×K	658.65	Joback Method
cpg	497.23	J/mol×K	695.48	Joback Method
cpg	511.93	J/mol×K	732.32	Joback Method
cpg	526.36	J/mol×K	769.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R279435&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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