cis-7,8-Epoxy-2-methyl-2-octadecene

Inchi: InChI=1S/C19H36O/c1-4-5-6-7-8-9-10-11-15-18-19(20-18)16-13-12-14-17(2)3/h14,18-19
InchiKey: XMPLISOJJFNIMC-UHFFFAOYSA-N
Formula: C19H36O
SMILES: CCCCCCCCCCC1OC1CCCC=C(C)C
Mol. weight [g/mol]: 280.49

Physical Properties

Property code	Value	Unit	Source
gf	147.69	kJ/mol	Joback Method
hf	-407.60	kJ/mol	Joback Method
hfus	51.04	kJ/mol	Joback Method
hvap	62.04	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.421		Crippen Method
mcvol	269.280	ml/mol	McGowan Method
pc	1191.52	kPa	Joback Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
tb	667.18	K	Joback Method
tc	841.44	K	Joback Method
tf	325.12	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.85	J/mol×K	667.18	Joback Method
cpg	808.34	J/mol×K	696.22	Joback Method
cpg	827.88	J/mol×K	725.27	Joback Method
cpg	846.51	J/mol×K	754.31	Joback Method
cpg	864.28	J/mol×K	783.35	Joback Method
cpg	881.25	J/mol×K	812.39	Joback Method
cpg	897.46	J/mol×K	841.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R413615&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