cis-7,8-Epoxy-2-methyl-1-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/h18-19H,2
InchiKey: GGFHLGTYSJQDFL-UHFFFAOYSA-N
Formula: C19H36O
SMILES: C=C(C)CCCCC1OC1CCCCCCCCCC
Mol. weight [g/mol]: 280.49

Physical Properties

Property code	Value	Unit	Source
gf	155.31	kJ/mol	Joback Method
hf	-399.39	kJ/mol	Joback Method
hfus	49.56	kJ/mol	Joback Method
hvap	61.41	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.421		Crippen Method
mcvol	269.280	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
tb	659.70	K	Joback Method
tc	830.98	K	Joback Method
tf	328.44	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.09	J/mol×K	659.70	Joback Method
cpg	805.52	J/mol×K	688.25	Joback Method
cpg	825.02	J/mol×K	716.79	Joback Method
cpg	843.62	J/mol×K	745.34	Joback Method
cpg	861.37	J/mol×K	773.89	Joback Method
cpg	878.31	J/mol×K	802.43	Joback Method
cpg	894.48	J/mol×K	830.98	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=R413600&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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