

cis-7,8-epoxy-2-methyl-Z14-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/h6-7,17-1
InchiKey:	LAPLCAPLSOWYAX-SREVYHEPSA-N
Formula:	C19H36O
SMILES:	CCCC=CCCCCCC1OC1CCCCC(C)C
Mol. weight [g/mol]:	280.49

Physical Properties

Property code	Value	Unit	Source
gf	153.80	kJ/mol	Joback Method
hf	-403.09	kJ/mol	Joback Method
hfus	48.83	kJ/mol	Joback Method
hvap	61.57	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	6.277		Crippen Method
mcvol	269.280	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
rinpol	2020.00		NIST Webbook
tb	666.86	K	Joback Method
tc	841.46	K	Joback Method
tf	324.08	K	Joback Method
vc	1.050	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.54	J/molxK	666.86	Joback Method
cpg	809.13	J/molxK	695.96	Joback Method
cpg	828.75	J/molxK	725.06	Joback Method
cpg	847.45	J/molxK	754.16	Joback Method
cpg	865.28	J/molxK	783.26	Joback Method
cpg	882.29	J/molxK	812.36	Joback Method
cpg	898.52	J/molxK	841.46	Joback Method
dvisc	0.0030466	Paxs	324.08	Joback Method
dvisc	0.0014694	Paxs	381.21	Joback Method

dvisc	0.0008570	Paxs	438.34	Joback Method
dvisc	0.0005660	Paxs	495.47	Joback Method
dvisc	0.0004073	Paxs	552.60	Joback Method
dvisc	0.0003118	Paxs	609.73	Joback Method
dvisc	0.0002498	Paxs	666.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R413759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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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