

cis-7,8-epoxy-2-methyl-E3-octadecene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C19H36O/c1-4-5-6-7-8-9-10-11-15-18-19(20-18)16-13-12-14-17(2)3/h12,14,17

HQAIZRNFD MSTLW-WYMLVPIESA-N

C19H36O

CCCCCCCCCCC1OC1CCC=CC(C)C

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	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
tb	666.86	K	Joback Method
tc	841.46	K	Joback Method
tf	324.08	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.54	J/mol×K	666.86	Joback Method
cpg	809.13	J/mol×K	695.96	Joback Method
cpg	828.75	J/mol×K	725.06	Joback Method
cpg	847.45	J/mol×K	754.16	Joback Method
cpg	865.28	J/mol×K	783.26	Joback Method
cpg	882.29	J/mol×K	812.36	Joback Method
cpg	898.52	J/mol×K	841.46	Joback Method
dvisc	0.0030466	Pa×s	324.08	Joback Method

dvisc	0.0014694	Pa×s	381.21	Joback Method
dvisc	0.0008570	Pa×s	438.34	Joback Method
dvisc	0.0005660	Pa×s	495.47	Joback Method
dvisc	0.0004073	Pa×s	552.60	Joback Method
dvisc	0.0003118	Pa×s	609.73	Joback Method
dvisc	0.0002498	Pa×s	666.86	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=R413695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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