

2-Methyl-Z-7,8-epoxyhexadecane

Other names:	2-(5-Methyl-hexyl)-3-octyl-oxirane
Inchi:	InChI=1S/C17H34O/c1-4-5-6-7-8-9-13-16-17(18-16)14-11-10-12-15(2)3/h15-17H,4-14H2
InchiKey:	QVIBKECDBFIZNV-UHFFFAOYSA-N
Formula:	C17H34O
SMILES:	CCCCCCCCC1OC1CCCCC(C)C
Mol. weight [g/mol]:	254.45

Physical Properties

Property code	Value	Unit	Source
gf	56.74	kJ/mol	Joback Method
hf	-479.03	kJ/mol	Joback Method
hfus	43.45	kJ/mol	Joback Method
hvap	57.16	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.721		Crippen Method
mcvol	245.400	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	1795.00		NIST Webbook
rinpol	1795.00		NIST Webbook
tb	616.94	K	Joback Method
tc	787.12	K	Joback Method
tf	306.62	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.87	J/mol×K	616.94	Joback Method
cpg	714.20	J/mol×K	645.30	Joback Method
cpg	733.62	J/mol×K	673.67	Joback Method
cpg	752.16	J/mol×K	702.03	Joback Method
cpg	769.87	J/mol×K	730.40	Joback Method
cpg	786.77	J/mol×K	758.76	Joback Method
cpg	802.89	J/mol×K	787.12	Joback Method

dvisc	0.0034590	Pa×s	306.62	Joback Method
dvisc	0.0017792	Pa×s	358.34	Joback Method
dvisc	0.0010823	Pa×s	410.06	Joback Method
dvisc	0.0007359	Pa×s	461.78	Joback Method
dvisc	0.0005408	Pa×s	513.50	Joback Method
dvisc	0.0004205	Pa×s	565.22	Joback Method
dvisc	0.0003410	Pa×s	616.94	Joback Method

Sources

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=U130863&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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