

1,11,14-Heptadecatriene, 8,9-epoxy, (Z)-

Inchi:	InChI=1S/C17H28O/c1-3-5-7-9-11-13-15-17-16(18-17)14-12-10-8-6-4-2/h4-5,7,11,13,16
InchiKey:	FQFKCVPCTWTEDI-KCPBOALRSA-N
Formula:	C17H28O
SMILES:	C=CCCCCCC1OC1CC=CCC=CCC
Mol. weight [g/mol]:	248.40

Physical Properties

Property code	Value	Unit	Source
gf	307.46	kJ/mol	Joback Method
hf	-113.88	kJ/mol	Joback Method
hfus	46.09	kJ/mol	Joback Method
hvap	56.80	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.193		Crippen Method
mcvol	232.500	ml/mol	McGowan Method
pc	1461.25	kPa	Joback Method
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
ripol	2235.00		NIST Webbook
ripol	2235.00		NIST Webbook
tb	622.38	K	Joback Method
tc	804.24	K	Joback Method
tf	309.70	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.54	J/molxK	622.38	Joback Method
cpg	650.39	J/molxK	652.69	Joback Method
cpg	668.28	J/molxK	683.00	Joback Method
cpg	685.26	J/molxK	713.31	Joback Method
cpg	701.40	J/molxK	743.62	Joback Method
cpg	716.75	J/molxK	773.93	Joback Method

cpg	731.38	J/molxK	804.24	Joback Method
dvisc	0.0021906	Paxs	309.70	Joback Method
dvisc	0.0012181	Paxs	361.81	Joback Method
dvisc	0.0007853	Paxs	413.93	Joback Method
dvisc	0.0005584	Paxs	466.04	Joback Method
dvisc	0.0004253	Paxs	518.15	Joback Method
dvisc	0.0003405	Paxs	570.27	Joback Method
dvisc	0.0002829	Paxs	622.38	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=R76210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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