1,8,14-Heptadecatriene, 11,12-epoxy

Inchi: InChI=1S/C17H28O/c1-3-5-7-8-9-10-11-13-15-17-16(18-17)14-12-6-4-2/h3,6,11-13,16-1
InchiKey: WNXISRDEAZBCKW-LWBHRHKWSA-N
Formula: C17H28O
SMILES: C=CCCCCCC=CCC1OC1CC=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	1815.00		NIST Webbook
rinpol	1815.00		NIST Webbook
ripol	2215.00		NIST Webbook
ripol	2215.00		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/mol×K	622.38	Joback Method
cpg	716.75	J/mol×K	773.93	Joback Method
cpg	701.40	J/mol×K	743.62	Joback Method
cpg	685.26	J/mol×K	713.31	Joback Method
cpg	668.28	J/mol×K	683.00	Joback Method
cpg	650.39	J/mol×K	652.69	Joback Method

cpg	731.38	J/mol×K	804.24	Joback Method
dvisc	0.0002829	Pa×s	622.38	Joback Method
dvisc	0.0003405	Pa×s	570.27	Joback Method
dvisc	0.0004253	Pa×s	518.15	Joback Method
dvisc	0.0005584	Pa×s	466.04	Joback Method
dvisc	0.0007853	Pa×s	413.93	Joback Method
dvisc	0.0012181	Pa×s	361.81	Joback Method
dvisc	0.0021906	Pa×s	309.70	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R76313&Units=SI

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