

1,11-Heptadecadiene, 8,9-epoxy

Inchi:	InChI=1S/C17H30O/c1-3-5-7-9-11-13-15-17-16(18-17)14-12-10-8-6-4-2/h4,11,13,16-17H
InchiKey:	QKWIFEQLRBYFGJ-ACCUITESSA-N
Formula:	C17H30O
SMILES:	C=CCCCCCC1OC1CC=CCCCC
Mol. weight [g/mol]:	250.42

Physical Properties

Property code	Value	Unit	Source
gf	227.24	kJ/mol	Joback Method
hf	-231.10	kJ/mol	Joback Method
hfus	45.89	kJ/mol	Joback Method
hvap	56.84	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.417		Crippen Method
mcvol	236.800	ml/mol	McGowan Method
pc	1404.84	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
ripol	2180.00		NIST Webbook
ripol	2180.00		NIST Webbook
tb	618.22	K	Joback Method
tc	793.91	K	Joback Method
tf	314.78	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.51	J/molxK	618.22	Joback Method
cpg	738.81	J/molxK	764.63	Joback Method
cpg	723.01	J/molxK	735.35	Joback Method
cpg	706.43	J/molxK	706.06	Joback Method
cpg	689.02	J/molxK	676.78	Joback Method
cpg	670.73	J/molxK	647.50	Joback Method

cpg	753.88	J/molxK	793.91	Joback Method
dvisc	0.0003274	Paxs	618.22	Joback Method
dvisc	0.0003940	Paxs	567.65	Joback Method
dvisc	0.0004917	Paxs	517.07	Joback Method
dvisc	0.0006439	Paxs	466.50	Joback Method
dvisc	0.0009001	Paxs	415.93	Joback Method
dvisc	0.0013808	Paxs	365.35	Joback Method
dvisc	0.0024302	Paxs	314.78	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=R76238&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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