

1,10,13-Hexadecatriene, 7,8-epoxy

Inchi:	InChI=1S/C16H26O/c1-3-5-7-9-10-12-14-16-15(17-16)13-11-8-6-4-2/h4-5,7,10,12,15-16
InchiKey:	LDGKUWWYKXNMRB-WRRYRWARSA-N
Formula:	C16H26O
SMILES:	C=CCCCC1OC1CC=CCC=CCC
Mol. weight [g/mol]:	234.38

Physical Properties

Property code	Value	Unit	Source
gf	299.04	kJ/mol	Joback Method
hf	-93.24	kJ/mol	Joback Method
hfus	43.50	kJ/mol	Joback Method
hvap	54.57	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.803		Crippen Method
mcvol	218.410	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinpol	1721.00		NIST Webbook
ripol	2128.00		NIST Webbook
tb	599.50	K	Joback Method
tc	782.96	K	Joback Method
tf	298.43	K	Joback Method
vc	0.850	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.57	J/molxK	599.50	Joback Method
cpg	596.09	J/molxK	630.08	Joback Method
cpg	613.64	J/molxK	660.65	Joback Method
cpg	630.28	J/molxK	691.23	Joback Method
cpg	646.07	J/molxK	721.81	Joback Method
cpg	661.07	J/molxK	752.38	Joback Method
cpg	675.35	J/molxK	782.96	Joback Method
dvisc	0.0021455	Paxs	298.43	Joback Method

dvisc	0.0012216	Paxs	348.61	Joback Method
dvisc	0.0008015	Paxs	398.79	Joback Method
dvisc	0.0005778	Paxs	448.97	Joback Method
dvisc	0.0004449	Paxs	499.14	Joback Method
dvisc	0.0003593	Paxs	549.32	Joback Method
dvisc	0.0003007	Paxs	599.50	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=R76185&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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