

1,11,14-Heptadecatriene, 8,9-dihydroxy

Inchi:	InChI=1S/C17H30O2/c1-3-5-7-9-11-13-15-17(19)16(18)14-12-10-8-6-4-2/h4-5,7,11,13,16
InchiKey:	PFODYVTXEFDXQP-KNVWVLGRSA-N
Formula:	C17H30O2
SMILES:	C=CCCCCCC(O)C(O)CC=CCC=CCC
Mol. weight [g/mol]:	266.42

Physical Properties

Property code	Value	Unit	Source
gf	62.02	kJ/mol	Joback Method
hf	-349.36	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	85.26	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.147		Crippen Method
mvol	249.230	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	1987.00		NIST Webbook
ripol	2899.00		NIST Webbook
tb	776.84	K	Joback Method
tc	955.34	K	Joback Method
tf	361.07	K	Joback Method
vc	0.955	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.05	J/molxK	776.84	Joback Method
cpg	764.60	J/molxK	806.59	Joback Method
cpg	778.49	J/molxK	836.34	Joback Method
cpg	791.75	J/molxK	866.09	Joback Method
cpg	804.44	J/molxK	895.84	Joback Method
cpg	816.61	J/molxK	925.59	Joback Method
cpg	828.32	J/molxK	955.34	Joback Method
dvisc	0.0090818	Paxs	361.07	Joback Method

dvisc	0.0008495	Paxs	430.37	Joback Method
dvisc	0.0001533	Paxs	499.66	Joback Method
dvisc	0.0000420	Paxs	568.95	Joback Method
dvisc	0.0000152	Paxs	638.25	Joback Method
dvisc	0.0000067	Paxs	707.54	Joback Method
dvisc	0.0000034	Paxs	776.84	Joback Method

Sources

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=R390597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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