

Oxirane, 5-hexenyl-

Other names:	7,8-Epoxy-1-octene 1-Octene, 7,8-epoxy- 1,2-Epoxy-7-octene 7,8-epoxyoctene
Inchi:	InChI=1S/C8H14O/c1-2-3-4-5-6-8-7-9-8/h2,8H,1,3-7H2
InchiKey:	UKTHULMXFLCNAV-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	C=CCCCC1CO1
Mol. weight [g/mol]:	126.20
CAS:	19600-63-6

Physical Properties

Property code	Value	Unit	Source
gf	78.95	kJ/mol	Joback Method
hf	-142.22	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	37.16	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.132		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	412.81	K	Joback Method
tc	594.99	K	Joback Method
tf	222.67	K	Joback Method
vc	0.443	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.15	J/mol×K	412.81	Joback Method
cpg	245.78	J/mol×K	443.17	Joback Method
cpg	258.70	J/mol×K	473.54	Joback Method
cpg	270.94	J/mol×K	503.90	Joback Method
cpg	282.53	J/mol×K	534.26	Joback Method

cpg	293.52	J/mol×K	564.62	Joback Method
cpg	303.92	J/mol×K	594.99	Joback Method
dvisc	0.0019220	Paxs	222.67	Joback Method
dvisc	0.0012922	Paxs	254.36	Joback Method
dvisc	0.0009486	Paxs	286.05	Joback Method
dvisc	0.0007407	Paxs	317.74	Joback Method
dvisc	0.0006049	Paxs	349.43	Joback Method
dvisc	0.0005109	Paxs	381.12	Joback Method
dvisc	0.0004429	Paxs	412.81	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=C19600636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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