Oxirane, hexadecyl-

Other names: 1,2-Epoxyoctadecane
Hexadecyl oxirane
Inchi: InChI=1S/C18H36O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-18-17-19-18/h18H,2-17H2
InchiKey: QBJWYMFTMJFGOL-UHFFFAOYSA-N
Formula: C18H36O
SMILES: CCCCCCCCCCCCCCCCC1CO1
Mol. weight [g/mol]: 268.48
CAS: 7390-81-0

Physical Properties

Property code	Value	Unit	Source
gf	75.31	kJ/mol	Joback Method
hf	-474.05	kJ/mol	Joback Method
hfus	48.49	kJ/mol	Joback Method
hvap	60.08	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	6.257		Crippen Method
mcvol	259.490	ml/mol	McGowan Method
pc	1253.03	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook
tb	644.93	K	Joback Method
tc	812.84	K	Joback Method
tf	337.13	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.85	J/mol×K	644.93	Joback Method
cpg	769.81	J/mol×K	672.92	Joback Method
cpg	788.88	J/mol×K	700.90	Joback Method
cpg	807.10	J/mol×K	728.89	Joback Method
cpg	824.50	J/mol×K	756.87	Joback Method

cpg	841.13	J/mol×K	784.86	Joback Method
cpg	857.02	J/mol×K	812.84	Joback Method
dvisc	0.0032727	Pa×s	337.13	Joback Method
dvisc	0.0016707	Pa×s	388.43	Joback Method
dvisc	0.0009977	Pa×s	439.73	Joback Method
dvisc	0.0006636	Pa×s	491.03	Joback Method
dvisc	0.0004768	Pa×s	542.33	Joback Method
dvisc	0.0003627	Pa×s	593.63	Joback Method
dvisc	0.0002882	Pa×s	644.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.20	K	0.07	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7390810&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume