Oxirane, butyl-

Other names:	1,2-epoxyhexane
	1,2-hexene oxide
	1-hexene epoxide
	1-hexene oxide
	2-butyloxirane
	Epoxy-n-hexane
	NSC 24268
	butyloxirane
	hexane, 1,2-epoxy-
Inchi:	InChI=1S/C6H12O/c1-2-3-4-6-5-7-6/h6H,2-5H2,1H3
InchiKey:	WHNBDXQTMPYBAT-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CCCCC1CO1
Mol. weight [g/mol]:	100.16
CAS:	1436-34-6

Physical Properties

Property code	Value	Unit	Source
gf	-25.73	kJ/mol	Joback Method
hf	-226.37	kJ/mol	Joback Method
hfus	17.41	kJ/mol	Joback Method
hvap	33.37	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.575		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	768.00		NIST Webbook
rinpol	768.00		NIST Webbook
tb	392.20	K	NIST Webbook
tc	550.63	K	Joback Method
tf	201.89	K	Joback Method
vc	0.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.67	J/mol×K	370.37	Joback Method
cpg	181.59	J/mol×K	400.41	Joback Method
cpg	192.91	J/mol×K	430.46	Joback Method
cpg	203.67	J/mol×K	460.50	Joback Method
cpg	213.89	J/mol×K	490.54	Joback Method
cpg	223.59	J/mol×K	520.58	Joback Method
cpg	232.79	J/mol×K	550.63	Joback Method
dvisc	0.0014937	Pa×s	201.89	Joback Method
dvisc	0.0010477	Pa×s	229.97	Joback Method
dvisc	0.0007938	Pa×s	258.05	Joback Method
dvisc	0.0006351	Pa×s	286.13	Joback Method
dvisc	0.0005288	Pa×s	314.21	Joback Method
dvisc	0.0004537	Pa×s	342.29	Joback Method
dvisc	0.0003985	Pa×s	370.37	Joback Method
hvapt	43.10	kJ/mol	345.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1436346&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Effect of anion species on infinite dilution activity coefficients of epoxides in imidazolium-based ionic liquids: https://www.doi.org/10.1016/j.fluid.2010.01.007

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

hvapt:	Enthalpy of vaporization at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume