Oxirane, ethyl-

Other names:	(.+/-.)-2-Ethyloxirane
	.alpha.-butylene oxide
	1,2-Butene oxide
	1,2-Butylene oxide
	1,2-EPOXYBUTANE
	1,2-Monoepoxybutane
	1,2-butylene epoxide
	1-Butene oxide
	1-Butylene oxide
	2-Ethyloxirane
	ALPHA-BUTYLENE OXIDE
	But-1-ene oxide
	Butane, 1,2-epoxy-
	Butylene oxide
	DL-1,2-Epoxybutane
	ETHYLETHYLENE OXIDE
	ETHYLOXIRANE
	Epoxybutane
	Ethylene oxide, ethyl-
	NCI-C55527
	NSC 24240
	Oxirane, 2-ethyl-
	butene 1,2-epoxide
	n-Butene-1,2-oxide
	«alpha»-Butylene oxide
	Â«alphaÂ»-Butylene oxide
Inchi:	InChI=1S/C4H8O/c1-2-4-3-5-4/h4H,2-3H2,1H3
InchiKey:	RBACIKXCRWGCBB-UHFFFAOYSA-N
Formula:	C4H8O
SMILES:	CCC1CO1
Mol. weight [g/mol]:	72.11
CAS:	106-88-7

Physical Properties

Property code	Value	Unit	Source
chl	-2548.50 ± 2.60	kJ/mol	NIST Webbook

gf	-42.57	kJ/mol	Joback Method
hf	-185.09	kJ/mol	Joback Method
hfl	-168.90 ± 2.60	kJ/mol	NIST Webbook
hfus	12.23	kJ/mol	Joback Method
hvap	28.92	kJ/mol	Joback Method
ie	10.15	eV	NIST Webbook
log10ws	-0.59		Crippen Method
logp	0.795		Crippen Method
mcvol	62.230	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
rinpol	582.00		NIST Webbook
rinpol	582.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	588.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	587.40		NIST Webbook
rinpol	587.80		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	551.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	571.00		NIST Webbook
rinpol	579.00		NIST Webbook
rinpol	574.00		NIST Webbook
rinpol	551.00		NIST Webbook
ripol	878.00		NIST Webbook
ripol	878.00		NIST Webbook
ripol	840.00		NIST Webbook
sg	324.03	J/mol×K	NIST Webbook
tb	336.50	K	NIST Webbook
tb	336.45	K	NIST Webbook
tb	335.90 ± 1.00	K	NIST Webbook
tb	334.00 ± 4.00	K	NIST Webbook
tc	505.23	K	Joback Method
tf	179.35	K	Joback Method
tt	143.87 ± 0.05	K	NIST Webbook
tt	143.87 ± 0.02	K	NIST Webbook
vc	0.237	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	101.12	J/mol×K	324.61	Joback Method
cpg	110.27	J/mol×K	354.71	Joback Method
cpg	118.93	J/mol×K	384.82	Joback Method
cpg	127.14	J/mol×K	414.92	Joback Method
cpg	134.91	J/mol×K	445.02	Joback Method
cpg	142.27	J/mol×K	475.13	Joback Method
cpg	149.22	J/mol×K	505.23	Joback Method
dvisc	0.0008071	Pa×s	179.35	Joback Method
dvisc	0.0006198	Pa×s	203.56	Joback Method
dvisc	0.0005035	Pa×s	227.77	Joback Method
dvisc	0.0004256	Pa×s	251.98	Joback Method
dvisc	0.0003706	Pa×s	276.19	Joback Method
dvisc	0.0003299	Pa×s	300.40	Joback Method
dvisc	0.0002989	Pa×s	324.61	Joback Method
hvapt	24.70	kJ/mol	300.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63613e+01
Coeff. B	-4.70155e+03
Coeff. C	6.38710e+01
Temperature range (K), min.	228.63
Temperature range (K), max.	361.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.85452e+01
Coeff. B	-5.18777e+03
Coeff. C	-4.95045e+00
Coeff. D	2.51404e-06

Temperature range (K), min.	123.15
Temperature range (K), max.	526.00

Sources

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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1046
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106887&Units=SI
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1046
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1046
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sg:	Molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume