Oxirane, (chloromethyl)-, (R)-

Other names: (2S)-chloromethyl-oxirane
(R)-(-)-Epichlorohydrin
Inchi: InChI=1S/C3H5ClO/c4-1-3-2-5-3/h3H,1-2H2/t3-/m1/s1
InchiKey: BRLQWZUYTZBJKN-GSVOUGTGSA-N
Formula: C3H5ClO
SMILES: ClCC1CO1
Mol. weight [g/mol]: 92.52
CAS: 51594-55-9

Physical Properties

Property code	Value	Unit	Source
gf	-62.92	kJ/mol	Joback Method
hf	-180.19	kJ/mol	Joback Method
hfus	13.84	kJ/mol	Joback Method
hvap	31.08	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	0.624		Crippen Method
mcvol	60.380	ml/mol	McGowan Method
pc	4945.39	kPa	Joback Method
tb	339.16	K	Joback Method
tc	530.37	K	Joback Method
tf	198.00	K	Joback Method
vc	0.231	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.88	J/mol×K	530.37	Joback Method
cpg	93.28	J/mol×K	339.16	Joback Method
cpg	100.62	J/mol×K	371.03	Joback Method
cpg	107.50	J/mol×K	402.90	Joback Method
cpg	113.95	J/mol×K	434.76	Joback Method
cpg	119.98	J/mol×K	466.63	Joback Method
cpg	125.61	J/mol×K	498.50	Joback Method

dvisc	0.0004154	Pa×s	339.16	Joback Method
dvisc	0.0011282	Pa×s	198.00	Joback Method
dvisc	0.0008743	Pa×s	221.53	Joback Method
dvisc	0.0007115	Pa×s	245.05	Joback Method
dvisc	0.0006004	Pa×s	268.58	Joback Method
dvisc	0.0005206	Pa×s	292.11	Joback Method
dvisc	0.0004612	Pa×s	315.63	Joback Method
rhol	1093.50	kg/m3	298.15	Enthalpic changes on mixing two couples of S- and R-enantiomers of benzyl-(1-phenyl-ethyl)-amine, 1-phenylethylamine, 1-phenyl-ethanol, butyric acid oxiranylmethyl ester, 4-methyl-[1,3]dioxolan-2-one, 2-chloro-methyloxirane and 3-hydroxyisobutyric acid methyl ester at T = 298.15 K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.70	K	48.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpic changes on mixing two couples of S- and R-enantiomers of benzyl-(1-phenyl-ethyl)-amine, 1-phenylethylamine, 1-phenyl-ethanol, butyric acid oxiranylmethyl ester, 4-methyl-[1,3]dioxolan-2-one, 2-chloro-methyloxirane and 3-hydroxyisobutyric acid methyl ester at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.10.019
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=C51594559&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
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume