2-chloroethyl chloroacetate

Other names: Ethanol, 2-chloro, chloroacetate
Inchi: InChI=1S/C4H6Cl2O2/c5-1-2-8-4(7)3-6/h1-3H2
InchiKey: XPUCYTFPMSEFIN-UHFFFAOYSA-N
Formula: C4H6Cl2O2
SMILES: O=C(CCl)OCCCl
Mol. weight [g/mol]: 157.00
CAS: 3848-12-2

Physical Properties

Property code	Value	Unit	Source
gf	-274.98	kJ/mol	Joback Method
hf	-402.17	kJ/mol	Joback Method
hfus	17.30	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	1.007		Crippen Method
mcvol	99.140	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	1002.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1016.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1803.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1759.00		NIST Webbook
tb	442.07	K	Joback Method
tc	636.71	K	Joback Method
tf	266.84	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.89	J/mol×K	636.71	Joback Method
cpg	202.53	J/mol×K	604.27	Joback Method
cpg	196.92	J/mol×K	571.83	Joback Method
cpg	191.05	J/mol×K	539.39	Joback Method
cpg	184.93	J/mol×K	506.95	Joback Method
cpg	178.56	J/mol×K	474.51	Joback Method
cpg	171.94	J/mol×K	442.07	Joback Method
dvisc	0.0028294	Pa×s	266.84	Joback Method
dvisc	0.0003546	Pa×s	442.07	Joback Method
dvisc	0.0004436	Pa×s	412.87	Joback Method
dvisc	0.0005740	Pa×s	383.66	Joback Method
dvisc	0.0007750	Pa×s	354.46	Joback Method
dvisc	0.0011043	Pa×s	325.25	Joback Method
dvisc	0.0016875	Pa×s	296.05	Joback Method
hvapt	53.30	kJ/mol	398.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3848122&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume