1-chloroethyl chloroacetate

Other names: Ethanol, 1-chloro, chloroacetate
Inchi: InChI=1S/C4H6Cl2O2/c1-3(6)8-4(7)2-5/h3H,2H2,1H3
InchiKey: MSULIXYJBOXXDR-UHFFFAOYSA-N
Formula: C4H6Cl2O2
SMILES: CC(Cl)OC(=O)CCl
Mol. weight [g/mol]: 157.00

Physical Properties

Property code	Value	Unit	Source
gf	-277.42	kJ/mol	Joback Method
hf	-407.45	kJ/mol	Joback Method
hfus	13.77	kJ/mol	Joback Method
hvap	42.04	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.353		Crippen Method
mcvol	99.140	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	910.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	926.00		NIST Webbook
ripol	1548.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1548.00		NIST Webbook
tb	441.63	K	Joback Method
tc	640.84	K	Joback Method
tf	251.84	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.11	J/mol×K	441.63	Joback Method
cpg	178.98	J/mol×K	474.83	Joback Method
cpg	185.57	J/mol×K	508.03	Joback Method
cpg	191.90	J/mol×K	541.23	Joback Method
cpg	197.95	J/mol×K	574.44	Joback Method
cpg	203.72	J/mol×K	607.64	Joback Method
cpg	209.22	J/mol×K	640.84	Joback Method
dvisc	0.0039286	Pa×s	251.84	Joback Method
dvisc	0.0020794	Pa×s	283.47	Joback Method
dvisc	0.0012506	Pa×s	315.10	Joback Method
dvisc	0.0008253	Pa×s	346.74	Joback Method
dvisc	0.0005838	Pa×s	378.37	Joback Method
dvisc	0.0004356	Pa×s	410.00	Joback Method
dvisc	0.0003390	Pa×s	441.63	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R112659&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume