2-chloroethyl dichloroacetate

Other names: Ethanol, 2-chloro, dichloroacetate
Inchi: InChI=1S/C4H5Cl3O2/c5-1-2-9-4(8)3(6)7/h3H,1-2H2
InchiKey: HSIYFNKETHDXJA-UHFFFAOYSA-N
Formula: C4H5Cl3O2
SMILES: O=C(OCCCl)C(Cl)Cl
Mol. weight [g/mol]: 191.44

Physical Properties

Property code	Value	Unit	Source
gf	-289.35	kJ/mol	Joback Method
hf	-423.19	kJ/mol	Joback Method
hfus	17.97	kJ/mol	Joback Method
hvap	46.42	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.572		Crippen Method
mcvol	111.380	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	1083.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1083.00		NIST Webbook
ripol	1846.00		NIST Webbook
ripol	1846.00		NIST Webbook
ripol	1866.00		NIST Webbook
ripol	1873.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1870.00		NIST Webbook
tb	479.06	K	Joback Method
tc	684.53	K	Joback Method
tf	281.76	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.28	J/mol×K	479.06	Joback Method
cpg	221.88	J/mol×K	650.28	Joback Method
cpg	216.57	J/mol×K	616.04	Joback Method
cpg	210.96	J/mol×K	581.79	Joback Method
cpg	205.04	J/mol×K	547.55	Joback Method
cpg	198.81	J/mol×K	513.30	Joback Method
cpg	226.88	J/mol×K	684.53	Joback Method
dvisc	0.0003417	Pa×s	479.06	Joback Method
dvisc	0.0004375	Pa×s	446.18	Joback Method
dvisc	0.0005827	Pa×s	413.29	Joback Method
dvisc	0.0008155	Pa×s	380.41	Joback Method
dvisc	0.0012163	Pa×s	347.53	Joback Method
dvisc	0.0019722	Pa×s	314.64	Joback Method
dvisc	0.0035797	Pa×s	281.76	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R112699&Units=SI

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