2-chloropropyl dichloroacetate

Other names: 1-Propanol, 2-chloro, dichloroacetate
Inchi: InChI=1S/C5H7Cl3O2/c1-3(6)2-10-5(9)4(7)8/h3-4H,2H2,1H3
InchiKey: FSUUBNKZAXHJPD-UHFFFAOYSA-N
Formula: C5H7Cl3O2
SMILES: CC(Cl)COC(=O)C(Cl)Cl
Mol. weight [g/mol]: 205.47

Physical Properties

Property code	Value	Unit	Source
gf	-283.37	kJ/mol	Joback Method
hf	-449.11	kJ/mol	Joback Method
hfus	17.04	kJ/mol	Joback Method
hvap	48.26	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.961		Crippen Method
mcvol	125.470	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	1089.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1117.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1810.00		NIST Webbook
ripol	1812.00		NIST Webbook
tb	501.50	K	Joback Method
tc	708.69	K	Joback Method
tf	278.03	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.57	J/mol×K	501.50	Joback Method
cpg	239.69	J/mol×K	536.03	Joback Method
cpg	247.40	J/mol×K	570.56	Joback Method
cpg	254.72	J/mol×K	605.10	Joback Method
cpg	261.64	J/mol×K	639.63	Joback Method
cpg	268.16	J/mol×K	674.16	Joback Method
cpg	274.29	J/mol×K	708.69	Joback Method
dvisc	0.0047788	Pa×s	278.03	Joback Method
dvisc	0.0022824	Pa×s	315.27	Joback Method
dvisc	0.0012744	Pa×s	352.52	Joback Method
dvisc	0.0007953	Pa×s	389.76	Joback Method
dvisc	0.0005389	Pa×s	427.01	Joback Method
dvisc	0.0003887	Pa×s	464.25	Joback Method
dvisc	0.0002943	Pa×s	501.50	Joback Method

Sources

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=R112555&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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