1-chloroethyl dichloroacetate

Other names: Ethanol, 1-chloro, dichloroacetate
Inchi: InChI=1S/C4H5Cl3O2/c1-2(5)9-4(8)3(6)7/h2-3H,1H3
InchiKey: XALCRQMVXZOFGU-UHFFFAOYSA-N
Formula: C4H5Cl3O2
SMILES: CC(Cl)OC(=O)C(Cl)Cl
Mol. weight [g/mol]: 191.44

Physical Properties

Property code	Value	Unit	Source
gf	-291.79	kJ/mol	Joback Method
hf	-428.47	kJ/mol	Joback Method
hfus	14.45	kJ/mol	Joback Method
hvap	46.03	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.918		Crippen Method
mcvol	111.380	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	980.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	979.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1611.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1594.00		NIST Webbook
tb	478.62	K	Joback Method
tc	688.86	K	Joback Method
tf	266.76	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.56	J/mol×K	478.62	Joback Method
cpg	199.32	J/mol×K	513.66	Joback Method
cpg	205.76	J/mol×K	548.70	Joback Method
cpg	211.87	J/mol×K	583.74	Joback Method
cpg	217.64	J/mol×K	618.78	Joback Method
cpg	223.09	J/mol×K	653.82	Joback Method
cpg	228.21	J/mol×K	688.86	Joback Method
dvisc	0.0049718	Pa×s	266.76	Joback Method
dvisc	0.0024180	Pa×s	302.07	Joback Method
dvisc	0.0013676	Pa×s	337.38	Joback Method
dvisc	0.0008616	Pa×s	372.69	Joback Method
dvisc	0.0005881	Pa×s	408.00	Joback Method
dvisc	0.0004265	Pa×s	443.31	Joback Method
dvisc	0.0003244	Pa×s	478.62	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R112664&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

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