1-chloroethyl trichloroacetate

Other names: Ethanol, 1-chloro, trichloroacetate
Inchi: InChI=1S/C4H4Cl4O2/c1-2(5)10-3(9)4(6,7)8/h2H,1H3
InchiKey: VYQBFWLIQIAUBR-UHFFFAOYSA-N
Formula: C4H4Cl4O2
SMILES: CC(Cl)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 225.88

Physical Properties

Property code	Value	Unit	Source
gf	-298.44	kJ/mol	Joback Method
hf	-447.68	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	49.51	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.485		Crippen Method
mcvol	123.620	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	1036.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1036.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1554.00		NIST Webbook
tb	513.26	K	Joback Method
tc	738.13	K	Joback Method
tf	314.10	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.59	J/mol×K	513.26	Joback Method
cpg	243.95	J/mol×K	700.65	Joback Method
cpg	239.23	J/mol×K	663.17	Joback Method
cpg	234.07	J/mol×K	625.69	Joback Method
cpg	228.42	J/mol×K	588.22	Joback Method
cpg	222.27	J/mol×K	550.74	Joback Method
cpg	248.23	J/mol×K	738.13	Joback Method
dvisc	0.0003143	Pa×s	513.26	Joback Method
dvisc	0.0004125	Pa×s	480.07	Joback Method
dvisc	0.0005637	Pa×s	446.87	Joback Method
dvisc	0.0008101	Pa×s	413.68	Joback Method
dvisc	0.0012400	Pa×s	380.49	Joback Method
dvisc	0.0020592	Pa×s	347.29	Joback Method
dvisc	0.0038064	Pa×s	314.10	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=R112679&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