2-chloropropyl trichloroacetate

Other names: 1-Propanol, 2-chloro, trichloroacetate
Inchi: InChI=1S/C5H6Cl4O2/c1-3(6)2-11-4(10)5(7,8)9/h3H,2H2,1H3
InchiKey: GXXHSZQJOWRTGY-UHFFFAOYSA-N
Formula: C5H6Cl4O2
SMILES: CC(Cl)COC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 239.91

Physical Properties

Property code	Value	Unit	Source
gf	-290.02	kJ/mol	Joback Method
hf	-468.32	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	51.74	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.527		Crippen Method
mcvol	137.710	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
rinpol	1217.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1210.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1778.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1794.00		NIST Webbook
ripol	1809.00		NIST Webbook
tb	536.14	K	Joback Method
tc	757.08	K	Joback Method
tf	325.37	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.96	J/mol×K	536.14	Joback Method
cpg	263.88	J/mol×K	572.96	Joback Method
cpg	271.22	J/mol×K	609.79	Joback Method
cpg	278.00	J/mol×K	646.61	Joback Method
cpg	284.24	J/mol×K	683.43	Joback Method
cpg	289.98	J/mol×K	720.26	Joback Method
cpg	295.24	J/mol×K	757.08	Joback Method
dvisc	0.0035419	Pa×s	325.37	Joback Method
dvisc	0.0018810	Pa×s	360.50	Joback Method
dvisc	0.0011178	Pa×s	395.63	Joback Method
dvisc	0.0007231	Pa×s	430.75	Joback Method
dvisc	0.0004995	Pa×s	465.88	Joback Method
dvisc	0.0003634	Pa×s	501.01	Joback Method
dvisc	0.0002757	Pa×s	536.14	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=R112560&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