3-chloropropyl dichloroacetate

Other names: 1-Propanol, 3-chloro, dichloroacetate
Inchi: InChI=1S/C5H7Cl3O2/c6-2-1-3-10-5(9)4(7)8/h4H,1-3H2
InchiKey: UFOHDQGORXKWPB-UHFFFAOYSA-N
Formula: C5H7Cl3O2
SMILES: O=C(OCCCCl)C(Cl)Cl
Mol. weight [g/mol]: 205.47

Physical Properties

Property code	Value	Unit	Source
gf	-280.93	kJ/mol	Joback Method
hf	-443.83	kJ/mol	Joback Method
hfus	20.56	kJ/mol	Joback Method
hvap	48.65	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.962		Crippen Method
mcvol	125.470	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1190.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1212.00		NIST Webbook
ripol	1923.00		NIST Webbook
ripol	1978.00		NIST Webbook
ripol	1971.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1923.00		NIST Webbook
ripol	1959.00		NIST Webbook
tb	501.94	K	Joback Method
tc	704.56	K	Joback Method
tf	293.03	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.25	J/mol×K	501.94	Joback Method
cpg	266.84	J/mol×K	670.79	Joback Method
cpg	260.47	J/mol×K	637.02	Joback Method
cpg	253.73	J/mol×K	603.25	Joback Method
cpg	246.61	J/mol×K	569.48	Joback Method
cpg	239.12	J/mol×K	535.71	Joback Method
cpg	272.85	J/mol×K	704.56	Joback Method
dvisc	0.0003111	Pa×s	501.94	Joback Method
dvisc	0.0004006	Pa×s	467.12	Joback Method
dvisc	0.0005371	Pa×s	432.30	Joback Method
dvisc	0.0007582	Pa×s	397.49	Joback Method
dvisc	0.0011435	Pa×s	362.67	Joback Method
dvisc	0.0018820	Pa×s	327.85	Joback Method
dvisc	0.0034866	Pa×s	293.03	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=R112580&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