5-chloropentyl dichloroacetate

Other names: 1-Pentanol, 5-chloro, dichloroacetate
Inchi: InChI=1S/C7H11Cl3O2/c8-4-2-1-3-5-12-7(11)6(9)10/h6H,1-5H2
InchiKey: CDYDOVYLGRVGGJ-UHFFFAOYSA-N
Formula: C7H11Cl3O2
SMILES: O=C(OCCCCCCl)C(Cl)Cl
Mol. weight [g/mol]: 233.52

Physical Properties

Property code	Value	Unit	Source
gf	-264.09	kJ/mol	Joback Method
hf	-485.11	kJ/mol	Joback Method
hfus	25.74	kJ/mol	Joback Method
hvap	53.10	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.742		Crippen Method
mcvol	153.650	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1440.00		NIST Webbook
ripol	2205.00		NIST Webbook
ripol	2215.00		NIST Webbook
ripol	2189.00		NIST Webbook
ripol	2182.00		NIST Webbook
tb	547.70	K	Joback Method
tc	744.75	K	Joback Method
tf	315.57	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.34	J/mol×K	547.70	Joback Method
cpg	361.00	J/mol×K	711.91	Joback Method

cpg	352.84	J/mol×K	679.07	Joback Method
cpg	344.20	J/mol×K	646.23	Joback Method
cpg	335.07	J/mol×K	613.38	Joback Method
cpg	325.45	J/mol×K	580.54	Joback Method
cpg	368.70	J/mol×K	744.75	Joback Method
dvisc	0.0002524	Pa×s	547.70	Joback Method
dvisc	0.0003280	Pa×s	509.01	Joback Method
dvisc	0.0004452	Pa×s	470.32	Joback Method
dvisc	0.0006382	Pa×s	431.63	Joback Method
dvisc	0.0009820	Pa×s	392.95	Joback Method
dvisc	0.0016604	Pa×s	354.26	Joback Method
dvisc	0.0031931	Pa×s	315.57	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R112471&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