2-chloropentyl dichloroacetate

Other names: 1-Pentanol, 2-chloro, dichloroacetate
Inchi: InChI=1S/C7H11Cl3O2/c1-2-3-5(8)4-12-7(11)6(9)10/h5-6H,2-4H2,1H3
InchiKey: ZPFQFDKDKWCBFM-UHFFFAOYSA-N
Formula: C7H11Cl3O2
SMILES: CCCC(Cl)COC(=O)C(Cl)Cl
Mol. weight [g/mol]: 233.52

Physical Properties

Property code	Value	Unit	Source
gf	-266.53	kJ/mol	Joback Method
hf	-490.39	kJ/mol	Joback Method
hfus	22.22	kJ/mol	Joback Method
hvap	52.71	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.741		Crippen Method
mcvol	153.650	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1322.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1313.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1952.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1958.00		NIST Webbook
ripol	1952.00		NIST Webbook
tb	547.26	K	Joback Method
tc	748.45	K	Joback Method
tf	300.57	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	315.72	J/mol×K	547.26	Joback Method
cpg	326.11	J/mol×K	580.79	Joback Method
cpg	335.97	J/mol×K	614.32	Joback Method
cpg	345.31	J/mol×K	647.85	Joback Method
cpg	354.14	J/mol×K	681.39	Joback Method
cpg	362.46	J/mol×K	714.92	Joback Method
cpg	370.28	J/mol×K	748.45	Joback Method
dvisc	0.0042701	Pa×s	300.57	Joback Method
dvisc	0.0019739	Pa×s	341.69	Joback Method
dvisc	0.0010770	Pa×s	382.80	Joback Method
dvisc	0.0006609	Pa×s	423.92	Joback Method
dvisc	0.0004421	Pa×s	465.03	Joback Method
dvisc	0.0003157	Pa×s	506.14	Joback Method
dvisc	0.0002372	Pa×s	547.26	Joback Method

Sources

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=R112382&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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