Dichloroacetic acid, pentyl ester

Other names:	1-Pentanol, dichloroacetate
	Pentyl dichloroacetate
Inchi:	InChI=1S/C7H12Cl2O2/c1-2-3-4-5-11-7(10)6(8)9/h6H,2-5H2,1H3
InchiKey:	UIFCHGLUUASAAI-UHFFFAOYSA-N
Formula:	C7H12Cl2O2
SMILES:	CCCCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]:	199.07
CAS:	37079-03-1

Physical Properties

Property code	Value	Unit	Source
gf	-252.16	kJ/mol	Joback Method
hf	-469.37	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	48.71	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.524		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1166.90		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1129.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1658.00		NIST Webbook
tb	510.27	K	Joback Method
tc	702.42	K	Joback Method
tf	285.65	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.96	J/mol×K	510.27	Joback Method
cpg	339.62	J/mol×K	670.39	Joback Method
cpg	330.81	J/mol×K	638.37	Joback Method
cpg	321.54	J/mol×K	606.34	Joback Method
cpg	311.82	J/mol×K	574.32	Joback Method
cpg	301.62	J/mol×K	542.29	Joback Method
cpg	347.98	J/mol×K	702.42	Joback Method
dvisc	0.0002658	Pa×s	510.27	Joback Method
dvisc	0.0003470	Pa×s	472.83	Joback Method
dvisc	0.0004742	Pa×s	435.40	Joback Method
dvisc	0.0006874	Pa×s	397.96	Joback Method
dvisc	0.0010763	Pa×s	360.52	Joback Method
dvisc	0.0018698	Pa×s	323.09	Joback Method
dvisc	0.0037541	Pa×s	285.65	Joback Method

Sources

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=C37079031&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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