Dichloroacetic acid, 2-pentyl ester

Other names: Acetic acid, dichloro, 1-methylbutyl ester
Inchi: InChI=1S/C7H12Cl2O2/c1-3-4-5(2)11-7(10)6(8)9/h5-6H,3-4H2,1-2H3
InchiKey: BSBLGRPLLFXELO-UHFFFAOYSA-N
Formula: C7H12Cl2O2
SMILES: CCCC(C)OC(=O)C(Cl)Cl
Mol. weight [g/mol]: 199.07
CAS: 90380-55-5

Physical Properties

Property code	Value	Unit	Source
gf	-254.60	kJ/mol	Joback Method
hf	-474.65	kJ/mol	Joback Method
hfus	18.02	kJ/mol	Joback Method
hvap	48.33	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.522		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1102.00		NIST Webbook
ripol	1504.00		NIST Webbook
tb	509.83	K	Joback Method
tc	706.13	K	Joback Method
tf	270.65	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.25	J/mol×K	509.83	Joback Method
cpg	302.21	J/mol×K	542.55	Joback Method
cpg	312.68	J/mol×K	575.26	Joback Method
cpg	322.65	J/mol×K	607.98	Joback Method
cpg	332.13	J/mol×K	640.70	Joback Method
cpg	341.13	J/mol×K	673.41	Joback Method

cpg	349.65	J/mol×K	706.13	Joback Method
dvisc	0.0052697	Pa×s	270.65	Joback Method
dvisc	0.0022910	Pa×s	310.51	Joback Method
dvisc	0.0012039	Pa×s	350.38	Joback Method
dvisc	0.0007215	Pa×s	390.24	Joback Method
dvisc	0.0004754	Pa×s	430.10	Joback Method
dvisc	0.0003363	Pa×s	469.97	Joback Method
dvisc	0.0002511	Pa×s	509.83	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=C90380555&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