Acetic acid, dichloro-, propyl ester

Other names:	Dichloroacetic acid, propyl ester
	1-Propanol, dichloroacetate
	Propyl dichloroacetate
Inchi:	InChI=1S/C5H8Cl2O2/c1-2-3-9-5(8)4(6)7/h4H,2-3H2,1H3
InchiKey:	AHRFMMRLDGAHBM-UHFFFAOYSA-N
Formula:	C5H8Cl2O2
SMILES:	CCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]:	171.02
CAS:	37587-81-8

Physical Properties

Property code	Value	Unit	Source
chl	-2636.00 ± 4.00	kJ/mol	NIST Webbook
chl	-2631.00	kJ/mol	NIST Webbook
gf	-269.00	kJ/mol	Joback Method
hf	-428.09	kJ/mol	Joback Method
hfus	16.36	kJ/mol	Joback Method
hvap	40.00	kJ/mol	NIST Webbook
log10ws	-1.69		Crippen Method
logp	1.743		Crippen Method
mcvol	113.230	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	974.50		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	934.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1471.00		NIST Webbook
ripol	1478.00		NIST Webbook
tb	464.51	K	Joback Method

tc	661.42	K	Joback Method
tf	263.11	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.55	J/mol×K	464.51	Joback Method
cpg	247.49	J/mol×K	628.60	Joback Method
cpg	240.59	J/mol×K	595.78	Joback Method
cpg	233.34	J/mol×K	562.97	Joback Method
cpg	225.76	J/mol×K	530.15	Joback Method
cpg	217.82	J/mol×K	497.33	Joback Method
cpg	254.06	J/mol×K	661.42	Joback Method
dvisc	0.0003158	Pa×s	464.51	Joback Method
dvisc	0.0004081	Pa×s	430.94	Joback Method
dvisc	0.0005509	Pa×s	397.38	Joback Method
dvisc	0.0007858	Pa×s	363.81	Joback Method
dvisc	0.0012050	Pa×s	330.24	Joback Method
dvisc	0.0020352	Pa×s	296.68	Joback Method
dvisc	0.0039296	Pa×s	263.11	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=C37587818&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
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

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