Dichloroacetic acid, 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

Physical Properties

Property code	Value	Unit	Source
chl	-2636.00 ± 4.00	kJ/mol	NIST Webbook
chl	-2631.00	kJ/mol	NIST Webbook
hf	-485.42	kJ/mol	Cheméo Relay (1.0)
hfus	16.36	kJ/mol	Joback Method
hvap	40.00	kJ/mol	NIST Webbook
ie	10.71	eV	Cheméo Relay (1.0)
log10ws	-1.64		Cheméo Relay (1.0)
logp	1.743		Crippen Method
mcvol	113.230	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	964.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	974.50		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	934.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1471.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1488.00		NIST Webbook
tb	441.34	K	Cheméo Relay (1.0)
tc	630.43	K	Cheméo Relay (1.0)

tf	222.59	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.55	J/mol×K	464.51	Joback Method
cpg	254.06	J/mol×K	661.42	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
dvisc	0.0007858	Pa×s	363.81	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	0.0039296	Pa×s	263.11	Joback Method
dvisc	0.0012050	Pa×s	330.24	Joback Method
dvisc	0.0020352	Pa×s	296.68	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37587818&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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