Chloroacetic acid, propyl ester

Other names:	Propyl chloroacetate
	Acetic acid, chloro-, propyl ester
Inchi:	InChI=1S/C5H9ClO2/c1-2-3-8-5(7)4-6/h2-4H2,1H3
InchiKey:	QJZNRCWAXUGABH-UHFFFAOYSA-N
Formula:	C5H9ClO2
SMILES:	CCCOC(=O)CCl
Mol. weight [g/mol]:	136.58
CAS:	5396-24-7

Physical Properties

Property code	Value	Unit	Source
chl	-2762.00 ± 2.00	kJ/mol	NIST Webbook
chl	-2761.90 ± 8.40	kJ/mol	NIST Webbook
chl	-2753.00	kJ/mol	NIST Webbook
gf	-254.63	kJ/mol	Joback Method
hf	-467.40 ± 4.60	kJ/mol	NIST Webbook
hfl	-516.00 ± 2.00	kJ/mol	NIST Webbook
hfus	15.69	kJ/mol	Joback Method
hvap	40.27	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	1.178		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	902.50		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	920.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1423.00		NIST Webbook
ripol	1419.00		NIST Webbook

ripol	1370.00		NIST Webbook
ripol	1381.00		NIST Webbook
tb	427.52	K	Joback Method
tc	613.54	K	Joback Method
tf	248.19	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.82	J/mol×K	427.52	Joback Method
cpg	195.11	J/mol×K	458.52	Joback Method
cpg	203.12	J/mol×K	489.53	Joback Method
cpg	210.84	J/mol×K	520.53	Joback Method
cpg	218.28	J/mol×K	551.53	Joback Method
cpg	225.43	J/mol×K	582.53	Joback Method
cpg	232.29	J/mol×K	613.54	Joback Method
dvisc	0.0016595	Pa×s	278.08	Joback Method
dvisc	0.0029404	Pa×s	248.19	Joback Method
dvisc	0.0010466	Pa×s	307.97	Joback Method
dvisc	0.0007162	Pa×s	337.86	Joback Method
dvisc	0.0005212	Pa×s	367.74	Joback Method
dvisc	0.0003979	Pa×s	397.63	Joback Method
dvisc	0.0003154	Pa×s	427.52	Joback Method
hfust	13.00	kJ/mol	240.00	NIST Webbook
hvapt	48.50	kJ/mol	293.00	NIST Webbook

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=C5396247&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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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