n-Propyl chloroformate

Other names:	Carbonochloridic acid, propyl ester
	Formic acid, chloro-, propyl ester
	Propyl chlorocarbonate
	Propyl chloroformate
	chloroformic acid propylester
	UN 2740
Inchi:	InChI=1S/C4H7ClO2/c1-2-3-7-4(5)6/h2-3H2,1H3
InchiKey:	QQKDTTWZXHEGAQ-UHFFFAOYSA-N
Formula:	C4H7ClO2
SMILES:	CCCOC(=O)Cl
Mol. weight [g/mol]:	122.55
CAS:	109-61-5

Physical Properties

Property code	Value	Unit	Source
gf	-263.05	kJ/mol	Joback Method
hf	-386.43	kJ/mol	Joback Method
hfl	-533.40 ± 0.76	kJ/mol	NIST Webbook
hfus	13.10	kJ/mol	Joback Method
hvap	40.70 ± 0.40	kJ/mol	NIST Webbook
hvap	40.70 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.49		Crippen Method
logp	1.772		Crippen Method
mcvol	86.900	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
rinpol	724.00		NIST Webbook
rinpol	724.00		NIST Webbook
tb	388.40	K	NIST Webbook
tb	387.35 ± 0.40	K	NIST Webbook
tb	378.70	K	NIST Webbook
tc	592.13	K	Joback Method
tf	236.92	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.10	J/mol×K	404.64	Joback Method
cpg	157.93	J/mol×K	435.89	Joback Method
cpg	164.55	J/mol×K	467.14	Joback Method
cpg	170.96	J/mol×K	498.39	Joback Method
cpg	177.14	J/mol×K	529.63	Joback Method
cpg	183.10	J/mol×K	560.88	Joback Method
cpg	188.84	J/mol×K	592.13	Joback Method
dvisc	0.0027868	Pa×s	236.92	Joback Method
dvisc	0.0016136	Pa×s	264.87	Joback Method
dvisc	0.0010371	Pa×s	292.83	Joback Method
dvisc	0.0007199	Pa×s	320.78	Joback Method
dvisc	0.0005298	Pa×s	348.73	Joback Method
dvisc	0.0004081	Pa×s	376.69	Joback Method
dvisc	0.0003259	Pa×s	404.64	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C109615&Units=SI

Legend

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume