1-Propanol, 3-chloro-, acetate

Other names:	«gamma»-Chloropropyl acetate
	3-Chloropropyl acetate
	3-Chloropropanol acetate
	3-Chlorprop-1-ylacetat
	1-Propanol, 3-chloro-, 1-acetate
Inchi:	InChI=1S/C5H9ClO2/c1-5(7)8-4-2-3-6/h2-4H2,1H3
InchiKey:	KPOHQIPNNIMWRL-UHFFFAOYSA-N
Formula:	C5H9ClO2
SMILES:	CC(=O)OCCCCl
Mol. weight [g/mol]:	136.58
CAS:	628-09-1

Physical Properties

Property code	Value	Unit	Source
gf	-254.63	kJ/mol	Joback Method
hf	-407.07	kJ/mol	Joback Method
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	922.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	895.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1418.00		NIST Webbook
ripol	1419.00		NIST Webbook
ripol	1414.00		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	0.0029404	Pa×s	248.19	Joback Method
dvisc	0.0016595	Pa×s	278.08	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.70	K	4.00	NIST Webbook

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=C628091&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume