1-Propanol, 1-chloro, acetate

Other names: 1-Chloropropyl acetate
Inchi: InChI=1S/C5H9ClO2/c1-3-5(6)8-4(2)7/h5H,3H2,1-2H3
InchiKey: VBEFTAAXOJJJKG-UHFFFAOYSA-N
Formula: C5H9ClO2
SMILES: CCC(Cl)OC(C)=O
Mol. weight [g/mol]: 136.58

Physical Properties

Property code	Value	Unit	Source
gf	-257.07	kJ/mol	Joback Method
hf	-412.35	kJ/mol	Joback Method
hfus	12.17	kJ/mol	Joback Method
hvap	39.88	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.524		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	821.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	806.00		NIST Webbook
ripol	1198.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1217.00		NIST Webbook
ripol	1222.00		NIST Webbook
ripol	1198.00		NIST Webbook
tb	427.08	K	Joback Method
tc	617.43	K	Joback Method
tf	233.19	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.92	J/mol×K	427.08	Joback Method
cpg	226.73	J/mol×K	585.71	Joback Method
cpg	219.39	J/mol×K	553.98	Joback Method
cpg	211.73	J/mol×K	522.26	Joback Method
cpg	203.77	J/mol×K	490.53	Joback Method
cpg	195.50	J/mol×K	458.81	Joback Method
cpg	233.77	J/mol×K	617.43	Joback Method
dvisc	0.0003024	Pa×s	427.08	Joback Method
dvisc	0.0003923	Pa×s	394.76	Joback Method
dvisc	0.0005332	Pa×s	362.45	Joback Method
dvisc	0.0007696	Pa×s	330.13	Joback Method
dvisc	0.0012028	Pa×s	297.82	Joback Method
dvisc	0.0020958	Pa×s	265.50	Joback Method
dvisc	0.0042591	Pa×s	233.19	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=R32955&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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