Ethanol, 1-chloro-, acetate

Other names: 1-Chloroethanol acetate
Inchi: InChI=1S/C4H7ClO2/c1-3(5)7-4(2)6/h3H,1-2H3
InchiKey: CGKKDGMMKSOGLM-UHFFFAOYSA-N
Formula: C4H7ClO2
SMILES: CC(=O)OC(C)Cl
Mol. weight [g/mol]: 122.55
CAS: 5912-58-3

Physical Properties

Property code	Value	Unit	Source
gf	-265.49	kJ/mol	Joback Method
hf	-391.71	kJ/mol	Joback Method
hfus	9.58	kJ/mol	Joback Method
hvap	37.65	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.134		Crippen Method
mcvol	86.900	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
rinpol	726.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	724.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1123.00		NIST Webbook
tb	404.20	K	Joback Method
tc	596.19	K	Joback Method
tf	221.92	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.16	J/mol×K	404.20	Joback Method
cpg	184.27	J/mol×K	564.19	Joback Method
cpg	178.13	J/mol×K	532.19	Joback Method
cpg	171.74	J/mol×K	500.19	Joback Method
cpg	165.11	J/mol×K	468.20	Joback Method
cpg	158.25	J/mol×K	436.20	Joback Method
cpg	190.17	J/mol×K	596.19	Joback Method
dvisc	0.0003140	Pa×s	404.20	Joback Method
dvisc	0.0004049	Pa×s	373.82	Joback Method
dvisc	0.0005462	Pa×s	343.44	Joback Method
dvisc	0.0007807	Pa×s	313.06	Joback Method
dvisc	0.0012051	Pa×s	282.68	Joback Method
dvisc	0.0020651	Pa×s	252.30	Joback Method
dvisc	0.0041012	Pa×s	221.92	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5912583&Units=SI
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

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