2-Chloroethyl propionate

Other names: Ethanol, 2-chloro-, propanoate
2-Chloroethyl propanoate
Inchi: InChI=1S/C5H9ClO2/c1-2-5(7)8-4-3-6/h2-4H2,1H3
InchiKey: VKSJVMZEQNIBNA-UHFFFAOYSA-N
Formula: C5H9ClO2
SMILES: CCC(=O)OCCCl
Mol. weight [g/mol]: 136.58
CAS: 1487-40-7

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	903.00		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

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=C1487407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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