

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
mvol	100.990	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinp	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.82	J/molxK	427.52	Joback Method
cpg	195.11	J/molxK	458.52	Joback Method
cpg	203.12	J/molxK	489.53	Joback Method
cpg	210.84	J/molxK	520.53	Joback Method
cpg	218.28	J/molxK	551.53	Joback Method
cpg	225.43	J/molxK	582.53	Joback Method

cpg	232.29	J/molxK	613.54	Joback Method
dvisc	0.0029404	Paxs	248.19	Joback Method
dvisc	0.0016595	Paxs	278.08	Joback Method
dvisc	0.0010466	Paxs	307.97	Joback Method
dvisc	0.0007162	Paxs	337.86	Joback Method
dvisc	0.0005212	Paxs	367.74	Joback Method
dvisc	0.0003979	Paxs	397.63	Joback Method
dvisc	0.0003154	Paxs	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/ci9903071
Crippen Method:	https://www.cheméo.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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