5-Chlorovaleric acid

Other names:	5-Chloro-n-valeric acid
	Pentanoic acid, 5-chloro-
Inchi:	InChI=1S/C5H9ClO2/c6-4-2-1-3-5(7)8/h1-4H2,(H,7,8)
InchiKey:	YSXDKDWNIPOSMF-UHFFFAOYSA-N
Formula:	C5H9ClO2
SMILES:	O=C(O)CCCCCl
Mol. weight [g/mol]:	136.58
CAS:	1119-46-6

Physical Properties

Property code	Value	Unit	Source
gf	-286.45	kJ/mol	Joback Method
hf	-427.08	kJ/mol	Joback Method
hfus	18.59	kJ/mol	Joback Method
hvap	54.53	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.480		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
rinpol	1174.00		NIST Webbook
tb	503.20	K	NIST Webbook
tc	675.67	K	Joback Method
tf	286.78	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.17	J/mol×K	497.28	Joback Method
cpg	240.12	J/mol×K	645.94	Joback Method
cpg	233.96	J/mol×K	616.21	Joback Method
cpg	227.50	J/mol×K	586.48	Joback Method
cpg	220.72	J/mol×K	556.74	Joback Method
cpg	213.61	J/mol×K	527.01	Joback Method

cpg	245.99	J/mol×K	675.67	Joback Method
dvisc	0.0002175	Pa×s	497.28	Joback Method
dvisc	0.0003395	Pa×s	462.20	Joback Method
dvisc	0.0005703	Pa×s	427.11	Joback Method
dvisc	0.0010511	Pa×s	392.03	Joback Method
dvisc	0.0021847	Pa×s	356.95	Joback Method
dvisc	0.0053264	Pa×s	321.86	Joback Method
dvisc	0.0161494	Pa×s	286.78	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=C1119466&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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