

# Chloromethyl 2-chlorohexanoate

<b>Other names:</b>	2-Chlorohexanoic acid, chloromethyl ester
<b>Inchi:</b>	InChI=1S/C7H12Cl2O2/c1-2-3-4-6(9)7(10)11-5-8/h6H,2-5H2,1H3
<b>InchiKey:</b>	SLCVMKYCEWYVKS-UHFFFAOYSA-N
<b>Formula:</b>	C7H12Cl2O2
<b>SMILES:</b>	CCCCC(Cl)C(=O)OCCI
<b>Mol. weight [g/mol]:</b>	199.07
<b>CAS:</b>	80418-53-7

## Physical Properties

Property code	Value	Unit	Source
gf	-252.16	kJ/mol	Joback Method
hf	-469.37	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	48.71	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.524		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1199.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1194.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1713.00		NIST Webbook
ripol	1733.00		NIST Webbook
tb	510.27	K	Joback Method
tc	702.42	K	Joback Method
tf	285.65	K	Joback Method
vc	0.543	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	290.96	J/molxK	510.27	Joback Method
cpg	339.62	J/molxK	670.39	Joback Method
cpg	330.81	J/molxK	638.37	Joback Method
cpg	321.54	J/molxK	606.34	Joback Method
cpg	311.82	J/molxK	574.32	Joback Method
cpg	301.62	J/molxK	542.29	Joback Method
cpg	347.98	J/molxK	702.42	Joback Method
dvisc	0.0002658	Paxs	510.27	Joback Method
dvisc	0.0003470	Paxs	472.83	Joback Method
dvisc	0.0004742	Paxs	435.40	Joback Method
dvisc	0.0006874	Paxs	397.96	Joback Method
dvisc	0.0010763	Paxs	360.52	Joback Method
dvisc	0.0018698	Paxs	323.09	Joback Method
dvisc	0.0037541	Paxs	285.65	Joback Method

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418537&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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