

# 2-Chlorohexanoic acid, methyl ester

<b>Other names:</b>	methyl 2-chlorohexanoate
<b>Inchi:</b>	InChI=1S/C7H13ClO2/c1-3-4-5-6(8)7(9)10-2/h6H,3-5H2,1-2H3
<b>InchiKey:</b>	ZKEGALQDZGNQIK-UHFFFAOYSA-N
<b>Formula:</b>	C7H13ClO2
<b>SMILES:</b>	CCCCC(Cl)C(=O)OC
<b>Mol. weight [g/mol]:</b>	164.63
<b>CAS:</b>	14925-60-1

## Physical Properties

Property code	Value	Unit	Source
gf	-240.23	kJ/mol	Joback Method
hf	-453.63	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	44.33	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.957		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	1047.00		NIST Webbook
ripol	1436.00		NIST Webbook
ripol	1436.00		NIST Webbook
ripol	1470.00		NIST Webbook
tb	472.84	K	Joback Method
tc	659.46	K	Joback Method
tf	255.73	K	Joback Method
vc	0.494	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.41	J/mol×K	472.84	Joback Method
cpg	316.63	J/mol×K	628.35	Joback Method
cpg	307.25	J/mol×K	597.25	Joback Method
cpg	297.44	J/mol×K	566.15	Joback Method

cpg	287.19	J/molxK	535.05	Joback Method
cpg	276.52	J/molxK	503.94	Joback Method
cpg	325.59	J/molxK	659.46	Joback Method
dvisc	0.0002680	Paxs	472.84	Joback Method
dvisc	0.0003514	Paxs	436.65	Joback Method
dvisc	0.0004840	Paxs	400.47	Joback Method
dvisc	0.0007104	Paxs	364.28	Joback Method
dvisc	0.0011348	Paxs	328.10	Joback Method
dvisc	0.0020358	Paxs	291.92	Joback Method
dvisc	0.0043091	Paxs	255.73	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C14925601&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14925601&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## 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
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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