

# Chloromethyl 2-chloroheptanoate

<b>Other names:</b>	2-Chloroheptanoic acid, chloromethyl ester
<b>Inchi:</b>	InChI=1S/C8H14Cl2O2/c1-2-3-4-5-7(10)8(11)12-6-9/h7H,2-6H2,1H3
<b>InchiKey:</b>	OEONJHNBIZMIO-UHFFFAOYSA-N
<b>Formula:</b>	C8H14Cl2O2
<b>SMILES:</b>	CCCCC(Cl)C(=O)OCCI
<b>Mol. weight [g/mol]:</b>	213.10
<b>CAS:</b>	80418-58-2

## Physical Properties

Property code	Value	Unit	Source
gf	-243.74	kJ/mol	Joback Method
hf	-490.01	kJ/mol	Joback Method
hfus	24.13	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.914		Crippen Method
mcvol	155.500	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1307.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1328.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1820.00		NIST Webbook
tb	533.15	K	Joback Method
tc	722.96	K	Joback Method
tf	296.92	K	Joback Method
vc	0.600	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.71	J/molxK	533.15	Joback Method
cpg	346.37	J/molxK	564.79	Joback Method
cpg	357.50	J/molxK	596.42	Joback Method
cpg	368.12	J/molxK	628.06	Joback Method
cpg	378.23	J/molxK	659.69	Joback Method
cpg	387.84	J/molxK	691.33	Joback Method
cpg	396.95	J/molxK	722.96	Joback Method
dvisc	0.0035993	Paxs	296.92	Joback Method
dvisc	0.0017614	Paxs	336.29	Joback Method
dvisc	0.0010012	Paxs	375.66	Joback Method
dvisc	0.0006335	Paxs	415.03	Joback Method
dvisc	0.0004339	Paxs	454.41	Joback Method
dvisc	0.0003157	Paxs	493.78	Joback Method
dvisc	0.0002408	Paxs	533.15	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418582&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418582&amp;Units=SI</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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