

# 7-Chloroheptanoic acid, methyl ester

<b>Other names:</b>	Heptanoic acid, 7-chloro, methyl ester
<b>Inchi:</b>	InChI=1S/C8H15ClO2/c1-11-8(10)6-4-2-3-5-7-9/h2-7H2,1H3
<b>InchiKey:</b>	YKSFGXAJDCLJKE-UHFFFAOYSA-N
<b>Formula:</b>	C8H15ClO2
<b>SMILES:</b>	COC(=O)CCCCCCI
<b>Mol. weight [g/mol]:</b>	178.66

## Physical Properties

Property code	Value	Unit	Source
gf	-229.37	kJ/mol	Joback Method
hf	-468.99	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	46.94	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.349		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1267.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1260.00		NIST Webbook
ripol	1799.00		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1842.00		NIST Webbook
tb	496.16	K	Joback Method
tc	677.00	K	Joback Method
tf	282.00	K	Joback Method
vc	0.556	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.66	J/mol×K	496.16	Joback Method

cpg	319.52	J/mol×K	526.30	Joback Method
cpg	330.91	J/mol×K	556.44	Joback Method
cpg	341.84	J/mol×K	586.58	Joback Method
cpg	352.32	J/mol×K	616.72	Joback Method
cpg	362.34	J/mol×K	646.86	Joback Method
cpg	371.92	J/mol×K	677.00	Joback Method
dvisc	0.0030458	Paxs	282.00	Joback Method
dvisc	0.0016080	Paxs	317.69	Joback Method
dvisc	0.0009658	Paxs	353.39	Joback Method
dvisc	0.0006370	Paxs	389.08	Joback Method
dvisc	0.0004506	Paxs	424.77	Joback Method
dvisc	0.0003363	Paxs	460.47	Joback Method
dvisc	0.0002618	Paxs	496.16	Joback Method

## Sources

<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=R91799&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R91799&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>

## 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

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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