

# 7-Chlorooctanoic acid, methyl ester

<b>Inchi:</b>	InChI=1S/C9H17ClO2/c1-8(10)6-4-3-5-7-9(11)12-2/h8H,3-7H2,1-2H3
<b>InchiKey:</b>	FPBIAFHTWMDMHC-UHFFFAOYSA-N
<b>Formula:</b>	C9H17ClO2
<b>SMILES:</b>	COC(=O)CCCCC(C)Cl
<b>Mol. weight [g/mol]:</b>	192.68

## Physical Properties

Property code	Value	Unit	Source
gf	-223.39	kJ/mol	Joback Method
hf	-494.91	kJ/mol	Joback Method
hfus	22.53	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.737		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	1316.00		NIST Webbook
rinpol	1308.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1775.00		NIST Webbook
tb	518.60	K	Joback Method
tc	701.32	K	Joback Method
tf	278.27	K	Joback Method
vc	0.607	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.38	J/molxK	518.60	Joback Method
cpg	412.64	J/molxK	670.86	Joback Method
cpg	401.64	J/molxK	640.41	Joback Method
cpg	390.13	J/molxK	609.96	Joback Method
cpg	378.08	J/molxK	579.51	Joback Method
cpg	365.50	J/molxK	549.05	Joback Method

cpg	423.11	J/molxK	701.32	Joback Method
dvisc	0.0002269	Paxs	518.60	Joback Method
dvisc	0.0003003	Paxs	478.55	Joback Method
dvisc	0.0004182	Paxs	438.49	Joback Method
dvisc	0.0006226	Paxs	398.44	Joback Method
dvisc	0.0010130	Paxs	358.38	Joback Method
dvisc	0.0018630	Paxs	318.32	Joback Method
dvisc	0.0040831	Paxs	278.27	Joback Method

## Sources

<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=R309789&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R309789&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>

## 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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