

# 3-Chloropropyl octanoate

<b>Other names:</b>	1-Propanol, 3-chloro, octanoate
<b>Inchi:</b>	InChI=1S/C11H21ClO2/c1-2-3-4-5-6-8-11(13)14-10-7-9-12/h2-10H2,1H3
<b>InchiKey:</b>	PEVLZFLWQKFZLP-UHFFFAOYSA-N
<b>Formula:</b>	C11H21ClO2
<b>SMILES:</b>	CCCCCCCC(=O)OCCCCI
<b>Mol. weight [g/mol]:</b>	220.74

## Physical Properties

Property code	Value	Unit	Source
gf	-204.11	kJ/mol	Joback Method
hf	-530.91	kJ/mol	Joback Method
hfus	31.23	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.519		Crippen Method
mvol	185.530	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
tb	564.80	K	Joback Method
tc	740.70	K	Joback Method
tf	315.81	K	Joback Method
vc	0.725	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.60	J/mol×K	564.80	Joback Method
cpg	460.98	J/mol×K	594.12	Joback Method
cpg	474.76	J/mol×K	623.43	Joback Method
cpg	487.95	J/mol×K	652.75	Joback Method
cpg	500.56	J/mol×K	682.07	Joback Method
cpg	512.59	J/mol×K	711.39	Joback Method
cpg	524.06	J/mol×K	740.70	Joback Method

dvisc	0.0027568	Paxs	315.81	Joback Method
dvisc	0.0013779	Paxs	357.31	Joback Method
dvisc	0.0007956	Paxs	398.81	Joback Method
dvisc	0.0005095	Paxs	440.30	Joback Method
dvisc	0.0003523	Paxs	481.80	Joback Method
dvisc	0.0002583	Paxs	523.30	Joback Method
dvisc	0.0001982	Paxs	564.80	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=R34315&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R34315&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>mvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-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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