

# 1-Propanol, 3-chloro, nonanoate

<b>Other names:</b>	3-Chloropropyl nonanoate
<b>Inchi:</b>	InChI=1S/C12H23ClO2/c1-2-3-4-5-6-7-9-12(14)15-11-8-10-13/h2-11H2,1H3
<b>InchiKey:</b>	ZLKLIVLFBLTYCO-UHFFFAOYSA-N
<b>Formula:</b>	C12H23ClO2
<b>SMILES:</b>	CCCCCCCCC(=O)OCCCCI
<b>Mol. weight [g/mol]:</b>	234.76

## Physical Properties

Property code	Value	Unit	Source
gf	-195.69	kJ/mol	Joback Method
hf	-551.55	kJ/mol	Joback Method
hfus	33.82	kJ/mol	Joback Method
hvap	55.85	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.909		Crippen Method
mvol	199.620	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1612.00		NIST Webbook
tb	587.68	K	Joback Method
tc	762.26	K	Joback Method
tf	327.08	K	Joback Method
vc	0.780	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.42	J/molxK	587.68	Joback Method
cpg	511.47	J/molxK	616.78	Joback Method
cpg	525.87	J/molxK	645.87	Joback Method
cpg	539.64	J/molxK	674.97	Joback Method
cpg	552.80	J/molxK	704.07	Joback Method
cpg	565.36	J/molxK	733.17	Joback Method
cpg	577.32	J/molxK	762.26	Joback Method
dvisc	0.0026085	Paxs	327.08	Joback Method

dvisc	0.0012830	Paxs	370.51	Joback Method
dvisc	0.0007323	Paxs	413.95	Joback Method
dvisc	0.0004650	Paxs	457.38	Joback Method
dvisc	0.0003194	Paxs	500.81	Joback Method
dvisc	0.0002330	Paxs	544.25	Joback Method
dvisc	0.0001781	Paxs	587.68	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R34301&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R34301&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>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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