

# 1-Propanol, 3-chloro, propanoate

<b>Other names:</b>	1-Propanol, 3-chloro, propionate
<b>Inchi:</b>	InChI=1S/C6H11ClO2/c1-2-6(8)9-5-3-4-7/h2-5H2,1H3
<b>InchiKey:</b>	HSOLEQBYEIZXJH-UHFFFAOYSA-N
<b>Formula:</b>	C6H11ClO2
<b>SMILES:</b>	CCC(=O)OCCCCl
<b>Mol. weight [g/mol]:</b>	150.60

## Physical Properties

Property code	Value	Unit	Source
gf	-246.21	kJ/mol	Joback Method
hf	-427.71	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	42.49	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.568		Crippen Method
mvol	115.080	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1016.00		NIST Webbook
rinpol	1016.00		NIST Webbook
tb	450.40	K	Joback Method
tc	634.77	K	Joback Method
tf	259.46	K	Joback Method
vc	0.445	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.90	J/mol×K	450.40	Joback Method
cpg	269.47	J/mol×K	604.04	Joback Method
cpg	261.25	J/mol×K	573.31	Joback Method
cpg	252.68	J/mol×K	542.58	Joback Method
cpg	243.77	J/mol×K	511.86	Joback Method
cpg	234.51	J/mol×K	481.13	Joback Method
cpg	277.34	J/mol×K	634.77	Joback Method

dvisc	0.0003003	Paxs	450.40	Joback Method
dvisc	0.0003813	Paxs	418.58	Joback Method
dvisc	0.0005036	Paxs	386.75	Joback Method
dvisc	0.0006992	Paxs	354.93	Joback Method
dvisc	0.0010354	Paxs	323.11	Joback Method
dvisc	0.0016707	Paxs	291.28	Joback Method
dvisc	0.0030315	Paxs	259.46	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R34333&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R34333&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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