

# Propanoic acid, 2-chloro, (Z)-3-hexenyl ester

<b>Inchi:</b>	InChI=1S/C9H15ClO2/c1-3-4-5-6-7-12-9(11)8(2)10/h4-5,8H,3,6-7H2,1-2H3/b5-4-
<b>InchiKey:</b>	YLEQBTXAXAMNEF-PLNGDYQASA-N
<b>Formula:</b>	C9H15ClO2
<b>SMILES:</b>	CCC=CCCOC(=O)C(C)Cl
<b>Mol. weight [g/mol]:</b>	190.67

## Physical Properties

Property code	Value	Unit	Source
gf	-143.17	kJ/mol	Joback Method
hf	-377.69	kJ/mol	Joback Method
hfus	22.73	kJ/mol	Joback Method
hvap	48.74	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.513		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1213.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1226.00		NIST Webbook
ripol	1637.00		NIST Webbook
ripol	1634.00		NIST Webbook
ripol	1645.00		NIST Webbook
tb	522.76	K	Joback Method
tc	713.52	K	Joback Method
tf	273.19	K	Joback Method
vc	0.587	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.35	J/molxK	522.76	Joback Method
cpg	391.96	J/molxK	681.73	Joback Method

cpg	381.57	J/molxK	649.93	Joback Method
cpg	370.63	J/molxK	618.14	Joback Method
cpg	359.13	J/molxK	586.35	Joback Method
cpg	347.04	J/molxK	554.55	Joback Method
cpg	401.81	J/molxK	713.52	Joback Method
dvisc	0.0001917	Paxs	522.76	Joback Method
dvisc	0.0002545	Paxs	481.16	Joback Method
dvisc	0.0003563	Paxs	439.57	Joback Method
dvisc	0.0005352	Paxs	397.98	Joback Method
dvisc	0.0008841	Paxs	356.38	Joback Method
dvisc	0.0016677	Paxs	314.78	Joback Method
dvisc	0.0038164	Paxs	273.19	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=R113805&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R113805&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>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point

**vc:** Critical Volume

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