

# 5-Chlorovaleric acid, octyl ester

<b>Inchi:</b>	InChI=1S/C13H25ClO2/c1-2-3-4-5-6-9-12-16-13(15)10-7-8-11-14/h2-12H2,1H3
<b>InchiKey:</b>	KWLSFBAAGRNDK-UHFFFAOYSA-N
<b>Formula:</b>	C13H25ClO2
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCCCl
<b>Mol. weight [g/mol]:</b>	248.79

## Physical Properties

Property code	Value	Unit	Source
gf	-187.27	kJ/mol	Joback Method
hf	-572.19	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	58.07	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.299		Crippen Method
mcvol	213.710	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinsol	1744.60		NIST Webbook
tb	610.56	K	Joback Method
tc	784.07	K	Joback Method
tf	338.35	K	Joback Method
vc	0.837	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.83	J/molxK	610.56	Joback Method
cpg	563.46	J/molxK	639.48	Joback Method
cpg	578.43	J/molxK	668.40	Joback Method
cpg	592.72	J/molxK	697.32	Joback Method
cpg	606.37	J/molxK	726.24	Joback Method
cpg	619.38	J/molxK	755.15	Joback Method
cpg	631.77	J/molxK	784.07	Joback Method
dvisc	0.0024461	Paxs	338.35	Joback Method
dvisc	0.0011849	Paxs	383.72	Joback Method

dvisc	0.0006691	Paxs	429.09	Joback Method
dvisc	0.0004215	Paxs	474.45	Joback Method
dvisc	0.0002878	Paxs	519.82	Joback Method
dvisc	0.0002089	Paxs	565.19	Joback Method
dvisc	0.0001590	Paxs	610.56	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=U292312&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292312&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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