

# 1-Hexanol, 5-chloro, acetate

**Inchi:** InChI=1S/C8H15ClO2/c1-7(9)5-3-4-6-11-8(2)10/h7H,3-6H2,1-2H3  
**InchiKey:** UDHQALRRQVPUTJ-UHFFFAOYSA-N  
**Formula:** C8H15ClO2  
**SMILES:** CC(=O)OCCCCC(C)Cl  
**Mol. weight [g/mol]:** 178.66

## Physical Properties

Property code	Value	Unit	Source
gf	-231.81	kJ/mol	Joback Method
hf	-474.27	kJ/mol	Joback Method
hfus	19.94	kJ/mol	Joback Method
hvap	46.55	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.347		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1171.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1194.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1650.00		NIST Webbook
tb	495.72	K	Joback Method
tc	680.38	K	Joback Method
tf	267.00	K	Joback Method
vc	0.550	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.89	J/molxK	495.72	Joback Method
cpg	363.91	J/molxK	649.60	Joback Method
cpg	353.67	J/molxK	618.82	Joback Method
cpg	342.95	J/molxK	588.05	Joback Method
cpg	331.75	J/molxK	557.27	Joback Method
cpg	320.07	J/molxK	526.50	Joback Method
cpg	373.67	J/molxK	680.38	Joback Method
dvisc	0.0002478	Paxs	495.72	Joback Method
dvisc	0.0003265	Paxs	457.60	Joback Method
dvisc	0.0004523	Paxs	419.48	Joback Method
dvisc	0.0006687	Paxs	381.36	Joback Method
dvisc	0.0010785	Paxs	343.24	Joback Method
dvisc	0.0019599	Paxs	305.12	Joback Method
dvisc	0.0042242	Paxs	267.00	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=R32820&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R32820&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
<b>vc:</b>	Critical Volume

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