

# 1-Octanol, 1-chloro, acetate

**Inchi:** InChI=1S/C10H19ClO2/c1-3-4-5-6-7-8-10(11)13-9(2)12/h10H,3-8H2,1-2H3  
**InchiKey:** FBXOZYBVABCPSH-UHFFFAOYSA-N  
**Formula:** C10H19ClO2  
**SMILES:** CCCCCCCC(Cl)OC(C)=O  
**Mol. weight [g/mol]:** 206.71

## Physical Properties

Property code	Value	Unit	Source
gf	-214.97	kJ/mol	Joback Method
hf	-515.55	kJ/mol	Joback Method
hfus	25.12	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.475		Crippen Method
mcvol	171.440	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1315.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1287.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1659.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1659.00		NIST Webbook
tb	541.48	K	Joback Method
tc	722.34	K	Joback Method
tf	289.54	K	Joback Method
vc	0.662	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.76	J/molxK	541.48	Joback Method
cpg	462.76	J/molxK	692.19	Joback Method
cpg	451.10	J/molxK	662.05	Joback Method
cpg	438.88	J/molxK	631.91	Joback Method
cpg	426.09	J/molxK	601.77	Joback Method
cpg	412.72	J/molxK	571.62	Joback Method
cpg	473.86	J/molxK	722.34	Joback Method
dvisc	0.0002061	Paxs	541.48	Joback Method
dvisc	0.0002738	Paxs	499.49	Joback Method
dvisc	0.0003832	Paxs	457.50	Joback Method
dvisc	0.0005741	Paxs	415.51	Joback Method
dvisc	0.0009417	Paxs	373.52	Joback Method
dvisc	0.0017512	Paxs	331.53	Joback Method
dvisc	0.0038985	Paxs	289.54	Joback Method

## Sources

<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=R32834&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R32834&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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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