

# 1-Undecanol, 6-chloro, acetate

<b>Other names:</b>	6-Chloroundecyl acetate
<b>Inchi:</b>	InChI=1S/C13H25ClO2/c1-3-4-6-9-13(14)10-7-5-8-11-16-12(2)15/h13H,3-11H2,1-2H3
<b>InchiKey:</b>	FYPRWZLMVSCPTN-UHFFFAOYSA-N
<b>Formula:</b>	C13H25ClO2
<b>SMILES:</b>	CCCCC(Cl)CCCCOC(C)=O
<b>Mol. weight [g/mol]:</b>	248.79

## Physical Properties

Property code	Value	Unit	Source
gf	-189.71	kJ/mol	Joback Method
hf	-577.47	kJ/mol	Joback Method
hfus	32.89	kJ/mol	Joback Method
hvap	57.69	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.298		Crippen Method
mcvol	213.710	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	1693.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1678.00		NIST Webbook
ripol	2166.00		NIST Webbook
ripol	2185.00		NIST Webbook
ripol	2159.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2177.00		NIST Webbook
tb	610.12	K	Joback Method
tc	786.44	K	Joback Method
tf	323.35	K	Joback Method
vc	0.831	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.21	J/mol×K	610.12	Joback Method
cpg	564.14	J/mol×K	639.51	Joback Method
cpg	579.37	J/mol×K	668.89	Joback Method
cpg	593.91	J/mol×K	698.28	Joback Method
cpg	607.77	J/mol×K	727.67	Joback Method
cpg	620.96	J/mol×K	757.05	Joback Method
cpg	633.51	J/mol×K	786.44	Joback Method
dvisc	0.0031957	Paxs	323.35	Joback Method
dvisc	0.0013781	Paxs	371.14	Joback Method
dvisc	0.0007200	Paxs	418.94	Joback Method
dvisc	0.0004297	Paxs	466.74	Joback Method
dvisc	0.0002822	Paxs	514.53	Joback Method
dvisc	0.0001991	Paxs	562.33	Joback Method
dvisc	0.0001484	Paxs	610.12	Joback Method

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R33836&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ripol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

**tb:** Normal Boiling Point Temperature  
**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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