

# 1-Octadecanol, 13-chloro, acetate

<b>Other names:</b>	13-Chlorooctadecyl acetate
<b>Inchi:</b>	InChI=1S/C20H39ClO2/c1-3-4-13-16-20(21)17-14-11-9-7-5-6-8-10-12-15-18-23-19(2)22
<b>InchiKey:</b>	ZZEWUEGFADWAQI-UHFFFAOYSA-N
<b>Formula:</b>	C20H39ClO2
<b>SMILES:</b>	CCCCC(Cl)CCCCCCCCCCCCOC(C)=O
<b>Mol. weight [g/mol]:</b>	346.98

## Physical Properties

Property code	Value	Unit	Source
gf	-130.77	kJ/mol	Joback Method
hf	-721.95	kJ/mol	Joback Method
hfus	51.02	kJ/mol	Joback Method
hvap	73.27	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	7.028		Crippen Method
mvol	312.340	ml/mol	McGowan Method
pc	1026.63	kPa	Joback Method
rinpol	2395.00		NIST Webbook
rinpol	2395.00		NIST Webbook
ripol	2903.00		NIST Webbook
ripol	2894.00		NIST Webbook
ripol	2894.00		NIST Webbook
tb	770.28	K	Joback Method
tc	948.76	K	Joback Method
tf	402.24	K	Joback Method
vc	1.222	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.69	J/mol×K	770.28	Joback Method
cpg	963.67	J/mol×K	800.03	Joback Method
cpg	981.68	J/mol×K	829.77	Joback Method
cpg	998.75	J/mol×K	859.52	Joback Method

cpg	1014.91	J/molxK	889.27	Joback Method
cpg	1030.18	J/molxK	919.02	Joback Method
cpg	1044.59	J/molxK	948.76	Joback Method
dvisc	0.0015827	Paxs	402.24	Joback Method
dvisc	0.0006361	Paxs	463.58	Joback Method
dvisc	0.0003163	Paxs	524.92	Joback Method
dvisc	0.0001821	Paxs	586.26	Joback Method
dvisc	0.0001164	Paxs	647.60	Joback Method
dvisc	0.0000804	Paxs	708.94	Joback Method
dvisc	0.0000589	Paxs	770.28	Joback Method

## Sources

<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=R33470&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R33470&amp;Units=SI</a>
<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>

## 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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