

# E-13-Octadecen-1-ol acetate

**Inchi:** InChI=1S/C20H38O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-20(2)21/h6-7H  
**InchiKey:** PPNRRQMJESAXGJ-VOTSOKGWSA-N  
**Formula:** C20H38O2  
**SMILES:** CCCCC=CCCCCCCCCCCCOC(C)=O  
**Mol. weight [g/mol]:** 310.51

## Physical Properties

Property code	Value	Unit	Source
gf	-36.18	kJ/mol	Joback Method
hf	-583.71	kJ/mol	Joback Method
hfus	50.54	kJ/mol	Joback Method
hvap	69.23	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.587		Crippen Method
mcvol	295.800	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
ripol	2200.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2045.00		NIST Webbook
tb	737.45	K	Joback Method
tc	911.93	K	Joback Method
tf	382.24	K	Joback Method
vc	1.159	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.45	J/molxK	737.45	Joback Method
cpg	972.40	J/molxK	882.85	Joback Method
cpg	956.69	J/molxK	853.77	Joback Method
cpg	940.17	J/molxK	824.69	Joback Method
cpg	922.81	J/molxK	795.61	Joback Method
cpg	904.58	J/molxK	766.53	Joback Method
cpg	987.32	J/molxK	911.93	Joback Method

dvisc	0.0000635	Paxs	737.45	Joback Method
dvisc	0.0000857	Paxs	678.25	Joback Method
dvisc	0.0001226	Paxs	619.05	Joback Method
dvisc	0.0001891	Paxs	559.84	Joback Method
dvisc	0.0003233	Paxs	500.64	Joback Method
dvisc	0.0006381	Paxs	441.44	Joback Method
dvisc	0.0015546	Paxs	382.24	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U130939&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U130939&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>
<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>

## 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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