

# E-12-hexadecenyl acetate

<b>Inchi:</b>	InChI=1S/C18H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-18(2)19/h5-6H,3-4,7
<b>InchiKey:</b>	MGPBZLCNYHCLEI-AATRIKPKSA-N
<b>Formula:</b>	C18H34O2
<b>SMILES:</b>	CCCC=CCCCCCCCCCCCOC(C)=O
<b>Mol. weight [g/mol]:</b>	282.46

## Physical Properties

Property code	Value	Unit	Source
gf	-53.02	kJ/mol	Joback Method
hf	-542.43	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	64.78	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.807		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
ripol	2328.00		NIST Webbook
ripol	2328.00		NIST Webbook
tb	691.69	K	Joback Method
tc	864.16	K	Joback Method
tf	359.70	K	Joback Method
vc	1.048	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.00	J/molxK	691.69	Joback Method
cpg	786.32	J/molxK	720.43	Joback Method
cpg	803.81	J/molxK	749.18	Joback Method
cpg	820.48	J/molxK	777.92	Joback Method
cpg	836.37	J/molxK	806.67	Joback Method
cpg	851.50	J/molxK	835.41	Joback Method

cpg	865.91	J/molxK	864.16	Joback Method
dvisc	0.0018910	Paxs	359.70	Joback Method
dvisc	0.0007915	Paxs	415.03	Joback Method
dvisc	0.0004066	Paxs	470.36	Joback Method
dvisc	0.0002403	Paxs	525.70	Joback Method
dvisc	0.0001570	Paxs	581.03	Joback Method
dvisc	0.0001105	Paxs	636.36	Joback Method
dvisc	0.0000822	Paxs	691.69	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=R86609&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R86609&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>ripol:</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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