

# (Z)-3-hexenyl undecanoate

Inchi:	InChI=1S/C17H32O2/c1-3-5-7-9-10-11-12-13-15-17(18)19-16-14-8-6-4-2/h6,8H,3-5,7,9-
InchiKey:	HLDPXZRNQXKWRH-VURMDHGXSA-N
Formula:	C17H32O2
SMILES:	CCC=CCCOC(=O)CCCCCCCCC
Mol. weight [g/mol]:	268.43

## Physical Properties

Property code	Value	Unit	Source
gf	-61.44	kJ/mol	Joback Method
hf	-521.79	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	62.55	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.417		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
ripol	2125.00		NIST Webbook
ripol	2125.00		NIST Webbook
tb	668.81	K	Joback Method
tc	841.03	K	Joback Method
tf	348.43	K	Joback Method
vc	0.992	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.95	J/molxK	668.81	Joback Method
cpg	728.86	J/molxK	697.51	Joback Method
cpg	745.96	J/molxK	726.22	Joback Method
cpg	762.28	J/molxK	754.92	Joback Method
cpg	777.84	J/molxK	783.62	Joback Method
cpg	792.67	J/molxK	812.33	Joback Method

cpg	806.79	J/molxK	841.03	Joback Method
dvisc	0.0020673	Paxs	348.43	Joback Method
dvisc	0.0008745	Paxs	401.83	Joback Method
dvisc	0.0004527	Paxs	455.22	Joback Method
dvisc	0.0002691	Paxs	508.62	Joback Method
dvisc	0.0001766	Paxs	562.02	Joback Method
dvisc	0.0001246	Paxs	615.41	Joback Method
dvisc	0.0000930	Paxs	668.81	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=R239868&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R239868&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>

## 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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