

# 12-Tridecen-2-yl acetate

<b>Inchi:</b>	InChI=1S/C15H28O2/c1-4-5-6-7-8-9-10-11-12-13-14(2)17-15(3)16/h4,14H,1,5-13H2,2-3H
<b>InchiKey:</b>	LKCYXFCSEWVFTO-UHFFFAOYSA-N
<b>Formula:</b>	C15H28O2
<b>SMILES:</b>	C=CCCCCCCCCCC(C)OC(C)=O
<b>Mol. weight [g/mol]:</b>	240.38

## Physical Properties

Property code	Value	Unit	Source
gf	-73.10	kJ/mol	Joback Method
hf	-477.58	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	57.08	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.635		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	1623.00		NIST Webbook
rinpol	1623.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1920.00		NIST Webbook
tb	615.13	K	Joback Method
tc	787.46	K	Joback Method
tf	314.21	K	Joback Method
vc	0.875	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.05	J/molxK	615.13	Joback Method
cpg	616.27	J/molxK	643.85	Joback Method
cpg	632.74	J/molxK	672.57	Joback Method
cpg	648.48	J/molxK	701.29	Joback Method
cpg	663.50	J/molxK	730.01	Joback Method
cpg	677.81	J/molxK	758.74	Joback Method

cpg	691.45	J/molxK	787.46	Joback Method
dvisc	0.0033107	Paxs	314.21	Joback Method
dvisc	0.0013405	Paxs	364.36	Joback Method
dvisc	0.0006755	Paxs	414.52	Joback Method
dvisc	0.0003947	Paxs	464.67	Joback Method
dvisc	0.0002561	Paxs	514.82	Joback Method
dvisc	0.0001794	Paxs	564.98	Joback Method
dvisc	0.0001332	Paxs	615.13	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=R203448&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R203448&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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