

# trans-Nerolidyl Acetate

<b>Other names:</b>	E-Nerolidyl acetate
<b>Inchi:</b>	InChI=1S/C17H28O2/c1-7-17(6,19-16(5)18)13-9-12-15(4)11-8-10-14(2)3/h7,10,12H,1,8-
<b>InchiKey:</b>	PRNJXUQTUSFYLV-NTCAYCPXSA-N
<b>Formula:</b>	C17H28O2
<b>SMILES:</b>	<chem>C=CC(C)(CCC=C(C)CCC=C(C)C)OC(C)=O</chem>
<b>Mol. weight [g/mol]:</b>	264.40
<b>CAS:</b>	85611-33-2

## Physical Properties

Property code	Value	Unit	Source
gf	92.36	kJ/mol	Joback Method
hf	-307.47	kJ/mol	Joback Method
hfus	31.66	kJ/mol	Joback Method
hvap	60.70	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.967		Crippen Method
mcvol	244.930	ml/mol	McGowan Method
pc	1446.83	kPa	Joback Method
rinpol	1715.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1713.00		NIST Webbook
tb	666.18	K	Joback Method
tc	858.25	K	Joback Method
tf	316.09	K	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.79	J/mol×K	666.18	Joback Method
cpg	685.72	J/mol×K	698.19	Joback Method
cpg	702.68	J/mol×K	730.20	Joback Method
cpg	718.71	J/mol×K	762.22	Joback Method
cpg	733.89	J/mol×K	794.23	Joback Method
cpg	748.27	J/mol×K	826.24	Joback Method
cpg	761.92	J/mol×K	858.25	Joback Method

## Sources

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C85611332&Units=SI>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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