

# (Z)-Nerolidol acetate

**Inchi:** InChI=1S/C16H26O2/c1-6-16(5,18-15(4)17)13-11-9-7-8-10-12-14(2)3/h6-7,9,12H,1,8,10  
**InchiKey:** OXQJDWZQDFSBHW-CLFYSBASSA-N  
**Formula:** C16H26O2  
**SMILES:** C=CC(C)(CCC=CCCC=C(C)C)OC(C)=O  
**Mol. weight [g/mol]:** 250.38

## Physical Properties

Property code	Value	Unit	Source
gf	92.49	kJ/mol	Joback Method
hf	-277.04	kJ/mol	Joback Method
hfus	30.38	kJ/mol	Joback Method
hvap	58.40	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.577		Crippen Method
mcvol	230.840	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1675.00		NIST Webbook
tb	643.42	K	Joback Method
tc	834.70	K	Joback Method
tf	318.78	K	Joback Method
vc	0.886	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	613.76	J/mol×K	643.42	Joback Method
cpg	631.14	J/mol×K	675.30	Joback Method
cpg	647.57	J/mol×K	707.18	Joback Method
cpg	663.09	J/mol×K	739.06	Joback Method
cpg	677.77	J/mol×K	770.94	Joback Method
cpg	691.67	J/mol×K	802.82	Joback Method
cpg	704.85	J/mol×K	834.70	Joback Method

## Sources

<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=R287986&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R287986&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## 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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-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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