

# Venlafaxine-M (nor-HO-)-H2O AC

**Inchi:** InChI=1S/C20H27NO4/c1-14(22)21(3)13-18(16-8-6-5-7-9-16)17-10-11-19(24-4)20(12-17)  
**InchiKey:** MFRJZPPOFJDWSW-UHFFFAOYSA-N  
**Formula:** C20H27NO4  
**SMILES:** COc1ccc(C(CN(C)C(C)=O)C2=CCCCC2)cc1OC(C)=O  
**Mol. weight [g/mol]:** 345.43

## Physical Properties

Property code	Value	Unit	Source
gf	-96.34	kJ/mol	Joback Method
hf	-548.92	kJ/mol	Joback Method
hfus	37.49	kJ/mol	Joback Method
hvap	85.37	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.683		Crippen Method
mvol	278.600	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	2560.00		NIST Webbook
rinpol	2560.00		NIST Webbook
tb	886.58	K	Joback Method
tc	1109.93	K	Joback Method
tf	553.31	K	Joback Method
vc	1.028	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.98	J/molxK	886.58	Joback Method
cpg	896.63	J/molxK	923.81	Joback Method
cpg	910.84	J/molxK	961.03	Joback Method
cpg	923.65	J/molxK	998.26	Joback Method
cpg	935.12	J/molxK	1035.48	Joback Method
cpg	945.26	J/molxK	1072.71	Joback Method
cpg	954.14	J/molxK	1109.93	Joback Method

# Sources

<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>
<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=R331236&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R331236&amp;Units=SI</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>hvp:</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>rinp:</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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