

# Clobazam M (norhydroxy-), hydrolysis, acetylated

<b>Inchi:</b>	InChI=1S/C18H17ClN2O4/c1-11(22)20-17-9-4-14(19)10-18(17)21(12(2)23)15-5-7-16(8-6
<b>InchiKey:</b>	VHYKZAOYNAVBFY-UHFFFAOYSA-N
<b>Formula:</b>	C18H17ClN2O4
<b>SMILES:</b>	CC(=O)Nc1ccc(Cl)cc1N(C(C)=O)c1ccc(OC(C)=O)cc1
<b>Mol. weight [g/mol]:</b>	360.79

## Physical Properties

Property code	Value	Unit	Source
gf	-6.91	kJ/mol	Joback Method
hf	-340.90	kJ/mol	Joback Method
hfus	47.59	kJ/mol	Joback Method
hvap	97.71	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.908		Crippen Method
mcvol	259.740	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook
tb	963.61	K	Joback Method
tc	1202.21	K	Joback Method
tf	670.09	K	Joback Method
vc	0.966	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.39	J/mol×K	963.61	Joback Method
cpg	771.34	J/mol×K	1003.38	Joback Method
cpg	780.12	J/mol×K	1043.14	Joback Method
cpg	787.81	J/mol×K	1082.91	Joback Method
cpg	794.45	J/mol×K	1122.68	Joback Method
cpg	800.10	J/mol×K	1162.45	Joback Method
cpg	804.83	J/mol×K	1202.21	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=R312864&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R312864&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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