

# Tetrazepam M (hydroxy-), isomer 3, hydrolysis, acetylated

<b>Inchi:</b>	InChI=1S/C18H20ClNO4/c1-11(21)20(3)17-8-7-14(19)10-16(17)18(23)13-5-4-6-15(9-13)
<b>InchiKey:</b>	AAOHXYJRPMOVEY-UHFFFAOYSA-N
<b>Formula:</b>	C18H20ClNO4
<b>SMILES:</b>	CC(=O)OC1CCC=C(C(=O)c2cc(Cl)ccc2N(C)C(C)=O)C1
<b>Mol. weight [g/mol]:</b>	349.81

## Physical Properties

Property code	Value	Unit	Source
gf	-154.30	kJ/mol	Joback Method
hf	-518.80	kJ/mol	Joback Method
hfus	41.51	kJ/mol	Joback Method
hvap	89.72	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.547		Crippen Method
mvol	258.360	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	2535.00		NIST Webbook
tb	905.47	K	Joback Method
tc	1139.86	K	Joback Method
tf	599.15	K	Joback Method
vc	0.958	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.20	J/mol×K	905.47	Joback Method
cpg	790.04	J/mol×K	944.54	Joback Method
cpg	801.52	J/mol×K	983.60	Joback Method
cpg	811.70	J/mol×K	1022.67	Joback Method
cpg	820.60	J/mol×K	1061.73	Joback Method
cpg	828.29	J/mol×K	1100.80	Joback Method
cpg	834.81	J/mol×K	1139.86	Joback Method

# Sources

<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=R313530&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R313530&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

# 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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