

# Nordazepam M (hydroxymethoxy-), hydrolysis, acetylated

<b>Inchi:</b>	InChI=1S/C18H16ClNO5/c1-10(21)20-16-7-4-12(19)8-15(16)18(23)14-6-5-13(24-3)9-17(
<b>InchiKey:</b>	ZNHUPRBLVNMYYTL-UHFFFAOYSA-N
<b>Formula:</b>	C18H16ClNO5
<b>SMILES:</b>	COc1ccc(C(=O)c2cc(Cl)ccc2NC(C)=O)c(OC(C)=O)c1
<b>Mol. weight [g/mol]:</b>	361.78

## Physical Properties

Property code	Value	Unit	Source
gf	-232.32	kJ/mol	Joback Method
hf	-552.12	kJ/mol	Joback Method
hfus	45.37	kJ/mol	Joback Method
hvap	98.74	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.463		Crippen Method
mvol	255.630	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	2990.00		NIST Webbook
rinpol	2990.00		NIST Webbook
tb	978.57	K	Joback Method
tc	1218.68	K	Joback Method
tf	672.37	K	Joback Method
vc	0.966	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.03	J/molxK	978.57	Joback Method
cpg	751.93	J/molxK	1018.59	Joback Method
cpg	759.46	J/molxK	1058.61	Joback Method
cpg	765.64	J/molxK	1098.62	Joback Method
cpg	770.48	J/molxK	1138.64	Joback Method
cpg	773.99	J/molxK	1178.66	Joback Method
cpg	776.20	J/molxK	1218.68	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=R313367&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R313367&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>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>rlnol:</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

Latest version available from:

<https://www.cheméo.com/cid/18-361-1/Nordazepam-M-hydroxymethoxy-hydrolysis-acetylated.pdf>

Generated by Cheméo on 2024-04-19 15:40:57.9960317 +0000 UTC m=+15830506.916609015.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.