

# Delorazepam M (hydroxy-), hydrolysis, acetylated

<b>Inchi:</b>	InChI=1S/C17H13Cl2NO4/c1-9(21)20-16-13(7-11(18)8-15(16)24-10(2)22)17(23)12-5-3-4
<b>InchiKey:</b>	KMUVYFBWIFHYHT-UHFFFAOYSA-N
<b>Formula:</b>	C17H13Cl2NO4
<b>SMILES:</b>	CC(=O)Nc1c(OC(C)=O)cc(Cl)cc1C(=O)c1cccc1Cl
<b>Mol. weight [g/mol]:</b>	366.19

## Physical Properties

Property code	Value	Unit	Source
gf	-147.67	kJ/mol	Joback Method
hf	-415.00	kJ/mol	Joback Method
hfus	45.79	kJ/mol	Joback Method
hvap	98.49	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.108		Crippen Method
mvol	247.910	ml/mol	McGowan Method
pc	2189.73	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	970.70	K	Joback Method
tc	1216.78	K	Joback Method
tf	668.79	K	Joback Method
vc	0.941	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.05	J/molxK	970.70	Joback Method
cpg	688.42	J/molxK	1011.71	Joback Method
cpg	695.62	J/molxK	1052.73	Joback Method
cpg	701.69	J/molxK	1093.74	Joback Method
cpg	706.66	J/molxK	1134.75	Joback Method
cpg	710.58	J/molxK	1175.77	Joback Method
cpg	713.47	J/molxK	1216.78	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R312973&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R312973&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.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>

# 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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