

# Clorazepate M (hydroxy-), isomer 2, hydrolysis, acetylated

<b>Inchi:</b>	InChI=1S/C17H14ClNO4/c1-10(20)19-16-8-5-13(18)9-15(16)17(22)12-3-6-14(7-4-12)23-
<b>InchiKey:</b>	YGHHKQDRXRDUHB-UHFFFAOYSA-N
<b>Formula:</b>	C17H14ClNO4
<b>SMILES:</b>	CC(=O)Nc1ccc(Cl)cc1C(=O)c1ccc(OC(C)=O)cc1
<b>Mol. weight [g/mol]:</b>	331.75

## Physical Properties

Property code	Value	Unit	Source
gf	-126.11	kJ/mol	Joback Method
hf	-387.79	kJ/mol	Joback Method
hfus	41.98	kJ/mol	Joback Method
hvap	93.44	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.455		Crippen Method
mcvol	235.670	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	2580.00		NIST Webbook
rinpol	2580.00		NIST Webbook
rinpol	2560.00		NIST Webbook
tb	928.29	K	Joback Method
tc	1170.75	K	Joback Method
tf	626.35	K	Joback Method
vc	0.891	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.39	J/molxK	928.29	Joback Method
cpg	674.16	J/molxK	968.70	Joback Method
cpg	682.76	J/molxK	1009.11	Joback Method
cpg	690.22	J/molxK	1049.52	Joback Method
cpg	696.60	J/molxK	1089.93	Joback Method
cpg	701.93	J/molxK	1130.34	Joback Method
cpg	706.25	J/molxK	1170.75	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=R312928&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R312928&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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