

# Clonazepam, M(amino-), acid hydrolyzed, acetylated

<b>Inchi:</b>	InChI=1S/C15H11ClN2O4/c1-9(19)17-14-7-6-10(18(21)22)8-12(14)15(20)11-4-2-3-5-13(
<b>InchiKey:</b>	KKAWPHZVPHAUPY-UHFFFAOYSA-N
<b>Formula:</b>	C15H11ClN2O4
<b>SMILES:</b>	CC(=O)Nc1ccc([N+](=O)[O-])cc1C(=O)c1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	318.71

## Physical Properties

Property code	Value	Unit	Source
gf	126.52	kJ/mol	Joback Method
hf	-112.47	kJ/mol	Joback Method
hfus	45.38	kJ/mol	Joback Method
hvap	96.43	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.438		Crippen Method
mvol	217.470	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	2845.00		NIST Webbook
rinpol	2845.00		NIST Webbook
tb	958.08	K	Joback Method
tc	1221.30	K	Joback Method
tf	675.26	K	Joback Method
vc	0.838	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.15	J/molxK	958.08	Joback Method
cpg	616.81	J/molxK	1001.95	Joback Method
cpg	624.44	J/molxK	1045.82	Joback Method
cpg	631.12	J/molxK	1089.69	Joback Method
cpg	636.94	J/molxK	1133.56	Joback Method
cpg	641.97	J/molxK	1177.43	Joback Method
cpg	646.31	J/molxK	1221.30	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=R255553&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R255553&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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