

# Lonazolac, hydroxy, bis-methylated

<b>Inchi:</b>	InChI=1S/C19H17ClN2O3/c1-24-15-9-5-13(6-10-15)19-21-16(11-17(23)25-2)18(22-19)1
<b>InchiKey:</b>	DSWWGKWTQCGBHZ-UHFFFAOYSA-N
<b>Formula:</b>	C19H17ClN2O3
<b>SMILES:</b>	<chem>COC(=O)CC1=NC(c2ccc(OC)cc2)N=C1c1ccc(Cl)cc1</chem>
<b>Mol. weight [g/mol]:</b>	356.80

## Physical Properties

Property code	Value	Unit	Source
gf	274.58	kJ/mol	Joback Method
hf	-83.09	kJ/mol	Joback Method
hfus	46.32	kJ/mol	Joback Method
hvap	94.30	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.854		Crippen Method
mcvol	257.100	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinsol	2875.00		NIST Webbook
tb	964.54	K	Joback Method
tc	1225.62	K	Joback Method
tf	686.62	K	Joback Method
vc	0.986	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.74	J/mol×K	964.54	Joback Method
cpg	816.42	J/mol×K	1008.05	Joback Method
cpg	824.87	J/mol×K	1051.57	Joback Method
cpg	831.09	J/mol×K	1095.08	Joback Method
cpg	835.06	J/mol×K	1138.59	Joback Method
cpg	836.79	J/mol×K	1182.11	Joback Method
cpg	836.25	J/mol×K	1225.62	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.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R201739&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R201739&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>hvap:</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>rinpola:</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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