

# Clonazepam, methylated

<b>Other names:</b>	Clonazepam, methyl
<b>Inchi:</b>	InChI=1S/C16H12ClN3O3/c1-19-14-7-6-10(20(22)23)8-12(14)16(18-9-15(19)21)11-4-2-3
<b>InchiKey:</b>	AZVBJJDUDXZLTM-UHFFFAOYSA-N
<b>Formula:</b>	C16H12ClN3O3
<b>SMILES:</b>	CN1C(=O)CN=C(c2ccccc2Cl)c2cc([N+](=O)[O-])ccc21
<b>Mol. weight [g/mol]:</b>	329.74

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	3.062		Crippen Method
mcvol	224.810	ml/mol	McGowan Method
rinpola	2766.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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=R41360&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R41360&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>

## Legend

<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>rinpola:</b>	Non-polar retention indices

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