

# Fludiazepam

<b>Other names:</b>	7-Chloro-5-(o-Fluorophenyl)-1,3-dihydro-1-methyl-2H-1,4-benzodiazepin-2-one Erispan ID-540 Ro-5-3438
<b>Inchi:</b>	InChI=1S/C16H12ClFN2O/c1-20-14-7-6-10(17)8-12(14)16(19-9-15(20)21)11-4-2-3-5-13
<b>InchiKey:</b>	ROYOYTLGLDIBX-UHFFFAOYSA-N
<b>Formula:</b>	C16H12ClFN2O
<b>SMILES:</b>	CN1C(=O)CN=C(c2ccccc2F)c2cc(Cl)ccc21
<b>Mol. weight [g/mol]:</b>	302.73
<b>CAS:</b>	3900-31-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	3.293		Crippen Method
mcpol	209.160	ml/mol	McGowan Method
rinpol	2389.00		NIST Webbook
rinpol	2408.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	2403.00		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=C3900310&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3900310&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>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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