

# 3H-1,4-benzodiazepine-2,5-dione, 7-chloro-1,2,4,5-tetrahydro-1,4-dimethyl-

Inchi:	InChI=1S/C11H11ClN2O2/c1-13-6-10(15)14(2)9-4-3-7(12)5-8(9)11(13)16/h3-5H,6H2,1-2
InchiKey:	CIMPFYWWMSFTPB-UHFFFAOYSA-N
Formula:	C11H11ClN2O2
SMILES:	CN1CC(=O)N(C)c2ccc(Cl)cc2C1=O
Mol. weight [g/mol]:	238.67
CAS:	1018-72-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	1.388		Crippen Method
mcvol	166.570	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1018720&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1018720&amp;Units=SI</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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