

# 1H-1,5-Benzodiazepine-2,4(3H,5H)-dione, 8-chloro-1-phenyl-

**Other names:** 8-Chloro-1-phenyl-1H-1,5-benzodiazepine-2,4(3H,5H)-dione

Desmethylclobazam

Norclobazam

Clofazin

**Inchi:** InChI=1S/C15H11ClN2O2/c16-10-6-7-12-13(8-10)18(11-4-2-1-3-5-11)15(20)9-14(19)17-

**InchiKey:** RRTVVRIKFKTKJK-UHFFFAOYSA-N

**Formula:** C15H11ClN2O2

**SMILES:** O=C1CC(=O)N(c2ccccc2)c2cc(Cl)ccc2N1

**Mol. weight [g/mol]:** 286.71

**CAS:** 22316-55-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Crippen Method
logp	3.347		Crippen Method
mcvol	199.170	ml/mol	McGowan Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C22316558&Units=SI>

## Legend

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

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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