

# N-Desmethyl-Zopiclone

**Inchi:** InChI=1S/C16H15ClN6O3/c17-10-1-2-11(21-9-10)23-14(24)12-13(20-4-3-19-12)15(23)2  
**InchiKey:** CGSFZSTXVVJLIX-UHFFFAOYSA-N  
**Formula:** C16H15ClN6O3  
**SMILES:** O=C(OC1c2nccnc2C(=O)N1c1ccc(Cl)cn1)N1CCNCC1  
**Mol. weight [g/mol]:** 374.78

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.73   |        | Crippen Method |
| logp          | 1.226   |        | Crippen Method |
| mcvol         | 248.190 | ml/mol | McGowan Method |
| rinpole       | 3089.00 |        | NIST Webbook   |
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## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R178491&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpole:** Non-polar retention indices

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