

# Clemizole, oxo

**Inchi:** InChI=1S/C19H18ClN3O/c20-15-9-7-14(8-10-15)13-23-17-6-2-1-5-16(17)21-18(23)19(24)  
**InchiKey:** GDXBQUOYJWFNE-UHFFFAOYSA-N  
**Formula:** C19H18ClN3O  
**SMILES:** O=C(c1nc2ccccc2n1Cc1ccc(Cl)cc1)N1CCCC1  
**Mol. weight [g/mol]:** 339.82

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.16   |        | Crippen Method |
| logp          | 3.974   |        | Crippen Method |
| mcvol         | 248.780 | ml/mol | McGowan Method |
| rinpol        | 2965.00 |        | NIST Webbook   |
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## Sources

**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R536288&Units=SI>

## 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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