

# Trimazosin

**Inchi:** InChI=1S/C20H29N5O6/c1-20(2,27)11-31-19(26)25-8-6-24(7-9-25)18-22-14-12(17(21)23)  
**InchiKey:** YNZXWQJZEDLQEG-UHFFFAOYSA-N  
**Formula:** C20H29N5O6  
**SMILES:** COc1cc2c(N)nc(N3CCN(C(=O)OCC(C)(C)O)CC3)nc2c(OC)c1OC  
**Mol. weight [g/mol]:** 435.48

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.64		Aqueous Solubility Prediction Method
log10ws	-3.64		Estimated Solubility Method
logp	1.267		Crippen Method
mcvol	319.400	ml/mol	McGowan Method

## Sources

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

## Legend

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

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