

# 4-Quinazolone, 3-methyl-2-pentyl

**Inchi:** InChI=1S/C14H18N2O/c1-3-4-5-10-13-15-12-9-7-6-8-11(12)14(17)16(13)2/h6-9H,3-5,10  
**InchiKey:** INNHMZODHHXQSL-UHFFFAOYSA-N  
**Formula:** C14H18N2O  
**SMILES:** CCCCCc1nc2ccccc2c(=O)n1C  
**Mol. weight [g/mol]:** 230.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.81		Crippen Method
logp	2.666		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook

## 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=R64603&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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