

# 4-Quinazolone, 2-pentyl

**Inchi:** InChI=1S/C13H16N2O/c1-2-3-4-9-12-14-11-8-6-5-7-10(11)13(16)15-12/h5-8H,2-4,9H2,1  
**InchiKey:** ZFDMQFNZNRCSQN-UHFFFAOYSA-N  
**Formula:** C13H16N2O  
**SMILES:** CCCCCc1nc2ccccc2c(=O)[nH]1  
**Mol. weight [g/mol]:** 216.28

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	2.174		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R64528&Units=SI>  
**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)

## 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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