

# 4-Quinazolone, 3-ethyl-2-propyl

**Inchi:** InChI=1S/C13H16N2O/c1-3-7-12-14-11-9-6-5-8-10(11)13(16)15(12)4-2/h5-6,8-9H,3-4,7H  
**InchiKey:** ZDTQDAVAHNPNGB-UHFFFAOYSA-N  
**Formula:** C13H16N2O  
**SMILES:** CCCc1nc2ccccc2c(=O)n1CC  
**Mol. weight [g/mol]:** 216.28

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	2.369		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
rinpol	1869.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1869.00		NIST Webbook

## Sources

**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=R64596&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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