

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

<b>Inchi:</b>	InChI=1S/C13H16N2O/c1-3-9-15-12(4-2)14-11-8-6-5-7-10(11)13(15)16/h5-8H,3-4,9H2,1
<b>InchiKey:</b>	ZIMFYUBAVNPVMC-UHFFFAOYSA-N
<b>Formula:</b>	C13H16N2O
<b>SMILES:</b>	CCc1c(CC)nc2ccccc2c1=O
<b>Mol. weight [g/mol]:</b>	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
rinpola	1873.00		NIST Webbook
rinpola	1873.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R64493&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R64493&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpola:</b>	Non-polar retention indices

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