

# 4(3H)-Quinazolinone, 3-methyl-

<b>Other names:</b>	3-Methyl-4-quinazolinone 4-Quinazolone, 3-methyl Quinazolin-4-one, 3-methyl
<b>Inchi:</b>	InChI=1S/C9H8N2O/c1-11-6-10-8-5-3-2-4-7(8)9(11)12/h2-6H,1H3
<b>InchiKey:</b>	FJVAQPINJBFBLI-UHFFFAOYSA-N
<b>Formula:</b>	C9H8N2O
<b>SMILES:</b>	Cn1cnc2ccccc2c1=O
<b>Mol. weight [g/mol]:</b>	160.17
<b>CAS:</b>	2436-66-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	0.933		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2436660&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2436660&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>rinpol:</b>	Non-polar retention indices

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