

# Quinoline, 5-(phenylazo)-

<b>Other names:</b>	Orotic acid, triTBDMS
<b>Inchi:</b>	InChI=1S/C15H11N3/c1-2-6-12(7-3-1)17-18-15-10-4-9-14-13(15)8-5-11-16-14/h1-11H
<b>InchiKey:</b>	RQIJYXYCHYDCDC-UHFFFAOYSA-N
<b>Formula:</b>	C15H11N3
<b>SMILES:</b>	<chem>c1ccc(N=Nc2cccc3ncccc23)cc1</chem>
<b>Mol. weight [g/mol]:</b>	233.27
<b>CAS:</b>	25117-46-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	4.650		Crippen Method
mcvol	180.870	ml/mol	McGowan Method
rinpola	2393.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C25117468&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25117468&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>
<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>rinpola:</b>	Non-polar retention indices

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