

# 5,8-Dihydro-2-methyl-3-(1-phenyl-5-tetrazolythio)

<b>Inchi:</b>	InChI=1S/C20H18N4O2S/c1-11-17(25)15-12-7-9-13(10-8-12)16(15)18(26)19(11)27-20-2
<b>InchiKey:</b>	BPFIAARDHLVVAX-UHFFFAOYSA-N
<b>Formula:</b>	C20H18N4O2S
<b>SMILES:</b>	<chem>Cc1c(O)c2c(c(O)c1Sc1nnnn1-c1ccccc1)C1C=CC2CC1</chem>
<b>Mol. weight [g/mol]:</b>	378.45
<b>CAS:</b>	5831-22-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.42		Crippen Method
logp	4.064		Crippen Method
mcvol	267.670	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5831221&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5831221&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>

## 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

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