

# 5-Methoxy-2(1-phenyl-5-mercaptotetrazole)-quinone

<b>Inchi:</b>	InChI=1S/C14H10N4O3S/c1-21-12-7-11(20)13(8-10(12)19)22-14-15-16-17-18(14)9-5-3-
<b>InchiKey:</b>	CGRQOOHXEFZOLT-UHFFFAOYSA-N
<b>Formula:</b>	C14H10N4O3S
<b>SMILES:</b>	<chem>COC1=CC(=O)C(Sc2nnnn2-c2ccccc2)=CC1=O</chem>
<b>Mol. weight [g/mol]:</b>	314.32
<b>CAS:</b>	95980-60-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	1.320		Crippen Method
mcvol	210.720	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C95980602&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C95980602&amp;Units=SI</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

Latest version available from:

<https://www.chemeo.com/cid/121-336-4/5-Methoxy-2-1-phenyl-5-mercaptotetrazole-quinone.pdf>

Generated by Cheméo on 2024-04-29 07:09:39.709565653 +0000 UTC m=+16663828.630142969.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.