

# Tioxolone

<b>Other names:</b>	6-Hydroxy-1,3-benzoxathiol-2-one 1,3-Benzoxathiol-2-one, 6-hydroxy- Thioxolone Camyna Stepin Thioxalone 6-Hydroxy-2-oxobenzoxathiole Acnosan
<b>Inchi:</b>	InChI=1S/C7H4O3S/c8-4-1-2-6-5(3-4)10-7(9)11-6/h1-3,8H
<b>InchiKey:</b>	SLYPOVJCSQHITR-UHFFFAOYSA-N
<b>Formula:</b>	C7H4O3S
<b>SMILES:</b>	O=c1oc2cc(O)ccc2s1
<b>Mol. weight [g/mol]:</b>	168.17
<b>CAS:</b>	4991-65-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.74		Crippen Method
logp	1.560		Crippen Method
mvol	104.530	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=C4991655&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4991655&amp;Units=SI</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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