

# 4'-Nitroflavone

<b>Inchi:</b>	InChI=1S/C15H9NO4/c17-13-9-15(20-14-4-2-1-3-12(13)14)10-5-7-11(8-6-10)16(18)19/h
<b>InchiKey:</b>	CKSVYVHLZNMXLX-UHFFFAOYSA-N
<b>Formula:</b>	C15H9NO4
<b>SMILES:</b>	O=c1cc(-c2ccc([N+](=O)[O-])cc2)oc2ccccc12
<b>Mol. weight [g/mol]:</b>	267.24
<b>CAS:</b>	19725-49-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.69		Crippen Method
logp	3.368		Crippen Method
mcvol	184.390	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=C19725496&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19725496&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

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