

# 4-Nitro-6H-dibenzo[b,d]pyran-6-one

<b>Inchi:</b>	InChI=1S/C13H7NO4/c15-13-10-5-2-1-4-8(10)9-6-3-7-11(14(16)17)12(9)18-13/h1-7H
<b>InchiKey:</b>	UGPKHPNHRLQNBO-UHFFFAOYSA-N
<b>Formula:</b>	C13H7NO4
<b>SMILES:</b>	O=c1oc2c([N+](=O)[O-])cccc2c2ccccc12
<b>Mol. weight [g/mol]:</b>	241.20

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.89		Crippen Method
logp	2.854		Crippen Method
mcvol	160.510	ml/mol	McGowan Method
rinpola	392.31		NIST Webbook

## 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=R175358&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R175358&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
<b>rinpola:</b>	Non-polar retention indices

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