

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

Inchi:	InChI=1S/C13H7NO4/c15-13-9-5-3-6-10(14(16)17)12(9)8-4-1-2-7-11(8)18-13/h1-7H
InchiKey:	WYNRQDVZADGTAY-UHFFFAOYSA-N
Formula:	C13H7NO4
SMILES:	O=c1oc2ccccc2c2c([N+](=O)[O-])cccc12
Mol. weight [g/mol]:	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
rinpol	399.84		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R175363&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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