

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

Inchi: InChI=1S/C13H7NO4/c15-13-10-4-2-1-3-9(10)11-7-8(14(16)17)5-6-12(11)18-13/h1-7H
InchiKey: NSXRBWUONVTXSK-UHFFFAOYSA-N
Formula: C13H7NO4
SMILES: O=c1oc2ccc([N+](=O)[O-])cc2c2ccccc12
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	385.15		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R175338&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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