

2-(3-Oxo-1,3-dihydro-2-benzofuran-1-yl)-1h-isoind

Inchi:	InChI=1S/C16H9NO4/c18-13-9-5-1-2-6-10(9)14(19)17(13)15-11-7-3-4-8-12(11)16(20)21
InchiKey:	ROOSRPSSNGBKTI-UHFFFAOYSA-N
Formula:	C16H9NO4
SMILES:	O=C1OC(N2C(=O)c3ccccc3C2=O)c2ccccc21
Mol. weight [g/mol]:	279.25
CAS:	101081-07-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	2.152		Crippen Method
mcvol	187.620	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C101081076&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/33-724-1/2-3-Oxo-1-3-dihydro-2-benzofuran-1-yl-1h-isoindole-1-3-2h-dione.pdf>

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