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