Dibenzo[d,d']benzodifuran

Inchi: InChI=1S/C14H8O2/c1-3-7-11-9(5-1)13-14(15-11)10-6-2-4-8-12(10)16-13/h1-8H
InchiKey: DYKMMHALDDEDOU-UHFFFAOYSA-N
Formula: C14H8O2
SMILES: c1ccc2c(c1)oc1c3ccccc3oc21
Mol. weight [g/mol]: 208.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.35		Crippen Method
logp	4.332		Crippen Method
mcvol	146.320	ml/mol	McGowan Method
rinpol	402.74		NIST Webbook
rinpol	407.65		NIST Webbook
rinpol	411.42		NIST Webbook
rinpol	402.74		NIST Webbook

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=R586040&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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