3-Phenyldibenzofuran

Inchi: InChI=1S/C18H12O/c1-2-6-13(7-3-1)14-10-11-16-15-8-4-5-9-17(15)19-18(16)12-14/h1-1
InchiKey: UWXLYSVMPRLLJW-UHFFFAOYSA-N
Formula: C18H12O
SMILES: c1ccc(-c2ccc3c(c2)oc2ccccc23)cc1
Mol. weight [g/mol]: 244.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.42		Crippen Method
logp	5.253		Crippen Method
mcvol	188.210	ml/mol	McGowan Method
rinpol	383.47		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=R556475&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