1-acetyl-4-methyl dibenzofuran

Inchi: InChI=1S/C15H12O2/c1-9-7-8-11(10(2)16)14-12-5-3-4-6-13(12)17-15(9)14/h3-8H,1-2H3
InchiKey: GWVDHRYHCOTEBJ-UHFFFAOYSA-N
Formula: C15H12O2
SMILES: CC(=O)c1ccc(C)c2oc3ccccc3c12
Mol. weight [g/mol]: 224.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.95		Crippen Method
logp	4.097		Crippen Method
mcvol	171.270	ml/mol	McGowan Method
rinpol	316.70		NIST Webbook
rinpol	296.17		NIST Webbook
rinpol	316.70		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R198148&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices