2-Furoic acid, 4-biphenyl ester

Inchi: InChI=1S/C17H12O3/c18-17(16-7-4-12-19-16)20-15-10-8-14(9-11-15)13-5-2-1-3-6-13/h1
InchiKey: ABTNYEMMMLVTBW-UHFFFAOYSA-N
Formula: C17H12O3
SMILES: O=C(Oc1ccc(-c2ccccc2)cc1)c1ccco1
Mol. weight [g/mol]: 264.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.90		Crippen Method
logp	4.166		Crippen Method
mcvol	196.720	ml/mol	McGowan Method
rinpol	2410.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U355177&Units=SI
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

Legend

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