

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
rinsol	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/ci9903071
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
rinsol:	Non-polar retention indices

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