

4,4'-Bis[2,2'-(4,4'-quinoline carboxylic acid)]biphenyl

Inchi:	InChI=1S/C32H20N2O4/c35-31(36)25-17-29(33-27-7-3-1-5-23(25)27)21-13-9-19(10-14-2
InchiKey:	NGTRRAPTKDQZIC-UHFFFAOYSA-N
Formula:	C32H20N2O4
SMILES:	O=C(O)c1cc(-c2ccc(-c3ccc(-c4cc(C(=O)O)c5ccccc5n4)cc3)cc2)nc2ccccc12
Mol. weight [g/mol]:	496.51
CAS:	4363-97-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.54		Crippen Method
logp	7.180		Crippen Method
mcvol	362.620	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4363977&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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