

2,11-Dibenzylbenzo[b]dipyrido[3,2,1-de:1,2,3-mn]-

Inchi:	InChI=1S/C36H24N2O2/c39-35-25(19-23-11-3-1-4-12-23)21-37-29-17-9-10-18-30(29)38
InchiKey:	KEAZBJPSWWRTMK-UHFFFAOYSA-N
Formula:	C36H24N2O2
SMILES:	O=c1c(Cc2ccccc2)cn2c3ccccc3n3cc(Cc4ccccc4)c(=O)c4c5ccccc5c1c2c43
Mol. weight [g/mol]:	516.59
CAS:	105564-86-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.27		Crippen Method
logp	6.991		Crippen Method
mcvol	385.520	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105564861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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