

3-Chloro-2-[(diphenoxyphosphoryl)oxy]-1,1'-biphenyl

Inchi:	InChI=1S/C24H18ClO4P/c25-23-18-10-17-22(19-11-4-1-5-12-19)24(23)29-30(26,27-20-
InchiKey:	JEULFOSBSAEBBO-UHFFFAOYSA-N
Formula:	C24H18ClO4P
SMILES:	O=P(Oc1ccccc1)(Oc1ccccc1)Oc1c(Cl)cccc1-c1ccccc1
Mol. weight [g/mol]:	436.82
CAS:	116295-52-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.43		Crippen Method
logp	7.652		Crippen Method
mcvol	310.160	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=C116295524&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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