Phosphoramidic acid, benzyl-, diphenyl ester

Other names:	diphenyl benzylphosphoramidate
Inchi:	InChI=1S/C19H18NO3P/c21-24(22-18-12-6-2-7-13-18,23-19-14-8-3-9-15-19)20-16-17-10
InchiKey:	WWOHGSPVWZHMKU-UHFFFAOYSA-N
Formula:	C19H18NO3P
SMILES:	O=P(NCc1ccccc1)(Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	339.32
CAS:	33985-75-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.50		Crippen Method
logp	5.042		Crippen Method
mcvol	255.340	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of Phosphoramidic Acid, N-(phenylmethyl)-, Diphenyl Ester in Selected Solvents:	https://www.doi.org/10.1021/acs.jced.5b00007
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33985750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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