Phosphorodiamidic acid, n,n'-diphenyl-, ethyl ester

Inchi: InChI=1S/C14H17N2O2P/c1-2-18-19(17,15-13-9-5-3-6-10-13)16-14-11-7-4-8-12-14/h3-1

InchiKey: QXSRXSXOXYIHBY-UHFFFAOYSA-N

Formula: C14H17N2O2P

SMILES: CCOP(=O)(Nc1ccccc1)Nc1ccccc1

Mol. weight [g/mol]: 276.27

CAS: 5586-09-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	4.355		Crippen Method
mcvol	212.760	ml/mol	McGowan Method

Sources

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=C5586094&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