Phosphoramidous acid,[p-(dimethylamino)phenyl]-,diethyl ester

Inchi: InChI=1S/C12H21N2O2P/c1-5-15-17(16-6-2)13-11-7-9-12(10-8-11)14(3)4/h7-10,13H,5-6

InchiKey: JJYUVRZLFFCBNK-UHFFFAOYSA-N

Formula: C12H21N2O2P

SMILES: CCOP(Nc1ccc(N(C)C)cc1)OCC

Mol. weight [g/mol]: 256.28

CAS: 5524-63-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.36		Crippen Method
logp	3.464		Crippen Method
mcvol	208.340	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5524630&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume