Phosphoro diamidic acid, n,n'-bis (2,4-dimethyl phenyl), ethyl ester

Inchi: InChI=1S/C18H25N2O2P/c1-6-22-23(21,19-17-9-7-13(2)11-15(17)4)20-18-10-8-14(3)12-16(18)5/h7-12H,6H2,1-5H3,(H2,19,20,21)

InchiKey: MXPYFDYSXONIRX-UHFFFAOYSA-N

Formula: C18H25N2O2P

SMILES: CCOP(=O)(Nc1ccc(C)cc1C)Nc1ccc(C)cc1C

Mol. weight [g/mol]: 332.38

CAS: 116401-84-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.39		Crippen Method
logp	5.589		Crippen Method
mcvol	269.120	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=C116401844&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