3-(4-N,N-Dimethylaminophenyl)propenoic acid, 2-(diethoxyphosphinyl)-, ethyl ester

Inchi: InChI=1S/C17H26NO5P/c1-6-21-17(19)12-10-14-9-11-15(18(4)5)13-16(14)24(20,22-7-2)

InchiKey: DIMUEXCWNYGPQE-ZRDIBKRKSA-N

Formula: C17H26NO5P

SMILES: CCOC(=O)C=Cc1ccc(N(C)C)cc1P(=O)(OCC)OCC

Mol. weight [g/mol]: 355.37

CAS: 66564-08-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.80		Crippen Method
logp	3.220		Crippen Method
mcvol	277.820	ml/mol	McGowan Method
ripol	2314.00		NIST Webbook
ripol	2314.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C66564087&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

ripol: Polar retention indices