

Phosphoramidous acid, 2,4-xylyl-, diethyl ester

Inchi:	InChI=1S/C12H20NO2P/c1-5-14-16(15-6-2)13-12-8-7-10(3)9-11(12)4/h7-9,13H,5-6H2,1-
InchiKey:	FZWUXZHNCUKIOZ-UHFFFAOYSA-N
Formula:	C12H20NO2P
SMILES:	CCOP(Nc1ccc(C)cc1C)OCC
Mol. weight [g/mol]:	241.27
CAS:	95845-11-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.69		Crippen Method
logp	4.015		Crippen Method
mcvol	198.360	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=C95845117&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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