

Phosphorodiamidic acid, n,n'-bis (p-n-butyl phenyl), ethyl ester

Inchi:	InChI=1S/C22H33N2O2P/c1-4-7-9-19-11-15-21(16-12-19)23-27(25,26-6-3)24-22-17-13-
InchiKey:	FBEABIJIPJQUNP-UHFFFAOYSA-N
Formula:	C22H33N2O2P
SMILES:	CCCCc1ccc(NP(=O)(Nc2ccc(CCCC)cc2)OCC)cc1
Mol. weight [g/mol]:	388.48
CAS:	116401-81-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.77		Crippen Method
logp	7.040		Crippen Method
mcvol	325.480	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116401811&Units=SI

Legend

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

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