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)24-22-17-13-2

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/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=C116401811&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume