Phosphoric triamide, n,n',n''-tri-p-dodecyl phenyl-

Inchi:	InChI=1S/C54H90N3OP/c1-4-7-10-13-16-19-22-25-28-31-34-49-37-43-52(44-38-49)55-5
InchiKey:	VWIOIKUKSPGPOB-UHFFFAOYSA-N
Formula:	C54H90N3OP
SMILES:	CCCCCCCCCCCCc1ccc(NP(=O)(Nc2ccc(CCCCCCCCCCCC)cc2)Nc2ccc(CCCCCCCC
Mol. weight [g/mol]:	828.29
CAS:	116295-70-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-21.77		Crippen Method
logp	18.821		Crippen Method
mcvol	756.710	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116295706&Units=SI
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

Legend

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

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