

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

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

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116295706&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116295706&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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