

Phosphoric triamide, n,n',n''-p-butyl phenyl-

Inchi:	InChI=1S/C30H42N3OP/c1-4-7-10-25-13-19-28(20-14-25)31-35(34,32-29-21-15-26(16-2
InchiKey:	QMRITVZUHUQEES-UHFFFAOYSA-N
Formula:	C30H42N3OP
SMILES:	CCCCc1ccc(NP(=O)(Nc2ccc(CCCC)cc2)Nc2ccc(CCCC)cc2)cc1
Mol. weight [g/mol]:	491.65
CAS:	98879-03-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.72		Crippen Method
logp	9.459		Crippen Method
mcvol	418.550	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98879039&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/78-106-8/Phosphoric-triamide-n-n-n-p-butyl-phenyl.pdf>

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