

Phosphoric triamide, n,n',n''-triphenyl-n,n',n''-trimethyl-

Inchi:	InChI=1S/C21H24N3OP/c1-22(19-13-7-4-8-14-19)26(25,23(2)20-15-9-5-10-16-20)24(3)2
InchiKey:	SXDAZEJYDNATRB-UHFFFAOYSA-N
Formula:	C21H24N3OP
SMILES:	CN(c1ccccc1)P(=O)(N(C)c1ccccc1)N(C)c1ccccc1
Mol. weight [g/mol]:	365.41
CAS:	50869-79-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.50		Crippen Method
logp	5.504		Crippen Method
mcvol	291.740	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=C50869799&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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