

Phosphoric triamide, n,n',n''-tris-(2,4-dimethyl phenyl)-

Inchi:	InChI=1S/C24H30N3OP/c1-16-7-10-22(19(4)13-16)25-29(28,26-23-11-8-17(2)14-20(23))
InchiKey:	WBEDASGBYSCFSL-UHFFFAOYSA-N
Formula:	C24H30N3OP
SMILES:	<chem>Cc1ccc(NP(=O)(Nc2ccc(C)cc2C)Nc2ccc(C)cc2C)c(C)c1</chem>
Mol. weight [g/mol]:	407.49
CAS:	116402-14-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.66		Crippen Method
logp	7.281		Crippen Method
mcvol	334.010	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116402143&Units=SI

Legend

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

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