

Phosphoric triamide, n,n',n''-tri-p-ethoxyphenyl-

Inchi:	InChI=1S/C24H30N3O4P/c1-4-29-22-13-7-19(8-14-22)25-32(28,26-20-9-15-23(16-10-20
InchiKey:	KCOXAWHMOVJZEBK-UHFFFAOYSA-N
Formula:	C24H30N3O4P
SMILES:	CCOc1ccc(NP(=O)(Nc2ccc(OCC)cc2)Nc2ccc(OCC)cc2)cc1
Mol. weight [g/mol]:	455.49
CAS:	116402-15-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.42		Crippen Method
logp	6.627		Crippen Method
mcvol	351.620	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=C116402154&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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