

Phosphonic diamide, n,n'-diphenyl

Inchi:	InChI=1S/C12H13N2OP/c15-16(13-11-7-3-1-4-8-11)14-12-9-5-2-6-10-12/h1-10,16H,(H2
InchiKey:	QUXAPACPSCALAA-UHFFFAOYSA-N
Formula:	C12H13N2OP
SMILES:	O=[PH](Nc1ccccc1)Nc1ccccc1
Mol. weight [g/mol]:	232.22
CAS:	4671-85-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	3.600		Crippen Method
mcvol	178.710	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=C4671856&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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