

Phenyl phosphazoanilide

Inchi:	InChI=1S/C12H11N2P/c1-3-7-11(8-4-1)13-15-14-12-9-5-2-6-10-12/h1-10H,(H,13,14)
InchiKey:	ZZRVACZASGFDFG-UHFFFAOYSA-N
Formula:	C12H11N2P
SMILES:	c1ccc(N=PNc2ccccc2)cc1
Mol. weight [g/mol]:	214.20
CAS:	5679-59-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.69		Crippen Method
logp	4.475		Crippen Method
mcvol	168.540	ml/mol	McGowan Method

Sources

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=C5679594&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/45-760-8/Phenyl-phosphazoanilide.pdf>

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