1,3,2-Diazaphosphorinane, 2-oxide, 2-phenoxy-

Inchi: InChI=1S/C9H13N2O2P/c12-14(10-7-4-8-11-14)13-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2,(H2

InchiKey: KHPUYXBDFOPCRF-UHFFFAOYSA-N

Formula: C9H13N2O2P

SMILES: O=P1(Oc2ccccc2)NCCCN1

Mol. weight [g/mol]: 212.19

CAS: 16456-52-3

Physical Properties

Property code	Value	Unit	Source
ie	8.29	eV	NIST Webbook
ie	9.43	eV	NIST Webbook
log10ws	-3.97		Crippen Method
logp	1.756		Crippen Method
mcvol	155.210	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=C16456523&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume