1,3,2-Diazaphosphole, 2-sulfide, 2-phenoxy-

Inchi: InChI=1S/C8H11N2OPS/c13-12(9-6-7-10-12)11-8-4-2-1-3-5-8/h1-5H,6-7H2,(H2,9,10,13)
InchiKey: FIKLAQMOIJQGIP-UHFFFAOYSA-N
Formula: C8H11N2OPS
SMILES: S=P1(Oc2ccccc2)NCCN1
Mol. weight [g/mol]: 214.22
CAS: 26387-49-5

Physical Properties

Property code	Value	Unit	Source
ie	8.09	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
log10ws	1.46		Crippen Method
logp	1.483		Crippen Method
mcvol	151.600	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C26387495&Units=SI

Legend

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