

1,3,2-Diazaphosphorinane, 2-sulfide, 2-phenoxy-

Inchi: InChI=1S/C9H13N2OPS/c14-13(10-7-4-8-11-13)12-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2,(H2)
InchiKey: CMJSRELZMBDESW-UHFFFAOYSA-N
Formula: C9H13N2OPS
SMILES: S=P1(Oc2ccccc2)NCCCN1
Mol. weight [g/mol]: 228.25
CAS: 26387-47-3

Physical Properties

Property code	Value	Unit	Source
ie	8.13	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
log10ws	1.04		Crippen Method
logp	1.873		Crippen Method
mcvol	165.690	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=C26387473&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

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