1,3,2-Diazaphosphepine, hexahydro-2-phenoxy 1-sulfide

Inchi: InChI=1S/C10H15N2OPS/c15-12-9-5-4-8-11-14(12)13-10-6-2-1-3-7-10/h1-3,6-7,11,15H,

InchiKey: KJQCJVYOYXUDTD-UHFFFAOYSA-N

Formula: C10H15N2OPS

SMILES: SN1CCCCNP1Oc1ccccc1

Mol. weight [g/mol]: 242.28

CAS: 26387-48-4

Physical Properties

Property code	Value	Unit	Source
ie	7.88	eV	NIST Webbook
ie	8.43	eV	NIST Webbook
log10ws	-0.39		Crippen Method
logp	2.822		Crippen Method
mcvol	179.780	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=C26387484&Units=SI

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

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume