

# 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](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/ci9903071>

## Legend

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

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