5,5-Dimethyl-2-phenoxy-1,3,2-dioxaphosphorinan 2-sulfide

Other names: 5,5-Dimethyl-2-phenoxy-1,3,2-dioxaphosphorinane 2-sulphide
Inchi: InChI=1S/C11H15O3PS/c1-11(2)8-12-15(16,13-9-11)14-10-6-4-3-5-7-10/h3-7H,8-9H2,1-
InchiKey: SLZVGNLFRUYWPW-UHFFFAOYSA-N
Formula: C11H15O3PS
SMILES: CC1(C)COP(=S)(Oc2ccccc2)OC1
Mol. weight [g/mol]: 258.27
CAS: 31951-84-5

Physical Properties

Property code	Value	Unit	Source
ie	8.30	eV	NIST Webbook
ie	9.15	eV	NIST Webbook
log10ws	0.65		Crippen Method
logp	3.363		Crippen Method
mcvol	185.650	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=C31951845&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

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