

5,5-Dimethyl-2-phenoxy-1,3,2-dioxaphosphorinane 2-sulphide

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]: 258.28

Physical Properties

Property code	Value	Unit	Source
ie	8.30	eV	NIST Webbook
ie	9.15	eV	NIST Webbook
logp	3.363		Crippen Method
mcvol	185.650	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C31951845&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/45-429-6/5-5-Dimethyl-2-phenoxy-1-3-2-dioxaphosphorinane-2-sulphide.pdf>

Generated by Cheméo on 2026-07-21 20:19:59.224458328 +0000 UTC m=+176295.066343725.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.