Phosphine oxide, dimethyl(3-methyl-1,2-butadienyl)-

Inchi: InChI=1S/C7H13OP/c1-7(2)5-6-9(3,4)8/h6H,1-4H3
InchiKey: VUWVTHXYNDTUOK-UHFFFAOYSA-N
Formula: C7H13OP
SMILES: CC(C)=C=CP(C)(C)=O
Mol. weight [g/mol]: 144.15
CAS: 68120-86-5

Physical Properties

Property code	Value	Unit	Source
ie	8.89	eV	NIST Webbook
log10ws	-3.27		Crippen Method
logp	2.688		Crippen Method
mcvol	127.220	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C68120865&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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

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