Phosphonic acid, (1,2-butadienyl-3-methyl), dimethyl ester

Inchi: InChI=1S/C7H13O3P/c1-7(2)5-6-11(8,9-3)10-4/h6H,1-4H3
InchiKey: NWKKSQUZYBRYCV-UHFFFAOYSA-N
Formula: C7H13O3P
SMILES: COP(=O)(C=C=C(C)C)OC
Mol. weight [g/mol]: 176.15
CAS: 4037-12-1

Physical Properties

Property code	Value	Unit	Source
ie	8.92	eV	NIST Webbook
log10ws	-3.42		Crippen Method
logp	2.551		Crippen Method
mcvol	138.960	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4037121&Units=SI

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.