Dimethyl allylphosphonate

Inchi: InChI=1S/C5H11O3P/c1-4-5-9(6,7-2)8-3/h4H,1,5H2,2-3H3
InchiKey: ZOSQAGGCVFVCNO-UHFFFAOYSA-N
Formula: C5H11O3P
SMILES: C=CCP(=O)(OC)OC
Mol. weight [g/mol]: 150.11
CAS: 757-54-0

Physical Properties

Property code	Value	Unit	Source
ie	9.96	eV	NIST Webbook
log10ws	-2.22		Crippen Method
logp	1.658		Crippen Method
mcvol	115.080	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=C757540&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.