

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: 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>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/38-602-1/Dimethyl-allylphosphonate.pdf>

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