

Allylphosphonic dichloride

Inchi: InChI=1S/C3H5Cl2OP/c1-2-3-7(4,5)6/h2H,1,3H2
InchiKey: LTHAMOYJECKDMD-UHFFFAOYSA-N
Formula: C3H5Cl2OP
SMILES: C=CCP(=O)(Cl)Cl
Mol. weight [g/mol]: 158.95
CAS: 1498-47-1

Physical Properties

Property code	Value	Unit	Source
ie	10.54	eV	NIST Webbook
log10ws	-3.51		Crippen Method
logp	2.843		Crippen Method
mcvol	99.640	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C1498471&Units=SI>

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/120-278-0/Allylphosphonic-dichloride.pdf>

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