

Phosphonic dichloride, 1,2-propadienyl-

Inchi: InChI=1S/C3H3Cl2OP/c1-2-3-7(4,5)6/h3H,1H2
InchiKey: VRXGHOPIMKAYJL-UHFFFAOYSA-N
Formula: C3H3Cl2OP
SMILES: C=C=CP(=O)(Cl)Cl
Mol. weight [g/mol]: 156.94
CAS: 17166-36-8

Physical Properties

Property code	Value	Unit	Source
ie	10.53	eV	NIST Webbook
log10ws	-3.88		Crippen Method
logp	2.956		Crippen Method
mcvol	95.340	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=C17166368&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/63-670-8/Phosphonic-dichloride-1-2-propadienyl.pdf>

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