

Phosphonothioic dichloride, ethenyl-

Inchi:	InChI=1S/C2H3Cl2PS/c1-2-5(3,4)6/h2H,1H2
InchiKey:	QDOPBBLWIUQTAW-UHFFFAOYSA-N
Formula:	C2H3Cl2PS
SMILES:	C=CP(=S)(Cl)Cl
Mol. weight [g/mol]:	160.99
CAS:	15849-99-7

Physical Properties

Property code	Value	Unit	Source
ie	9.70	eV	NIST Webbook
log10ws	1.42		Crippen Method
logp	2.917		Crippen Method
mcvol	96.030	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15849997&Units=SI
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

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/81-195-6/Phosphonothioic-dichloride-ethenyl.pdf>

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