Phosphenodithioic chloride

Inchi:	InChI=1S/ClPS2/c1-2(3)4
InchiKey:	FKUUPFFACLEMRI-UHFFFAOYSA-N
Formula:	ClPS2
SMILES:	S=P(=S)Cl
Mol. weight [g/mol]:	130.56
CAS:	67318-23-4

Physical Properties

Property code	Value	Unit	Source
ie	9.80	eV	NIST Webbook
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log10ws	3.44		Crippen Method
logp	1.546		Crippen Method
mcvol	71.960	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=C67318234&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/54-155-0/Phosphenodithioic-chloride.pdf

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