

Phosphenodithioic chloride

Inchi: InChI=1S/CIPS2/c1-2(3)4
InchiKey: FKUUPFFACLEMRI-UHFFFAOYSA-N
Formula: CIPS2
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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