

Thiophosphoryl chloride

Other names: thiophosphoryl trichloride
Inchi: InChI=1S/Cl3PS/c1-4(2,3)5
InchiKey: WQYSXVGEZYESBR-UHFFFAOYSA-N
Formula: Cl3PS
SMILES: S=P(Cl)(Cl)Cl
Mol. weight [g/mol]: 169.40
CAS: 3982-91-0

Physical Properties

Property code	Value	Unit	Source
ie	10.13 ± 0.03	eV	NIST Webbook
ie	9.71 ± 0.03	eV	NIST Webbook
ie	9.71 ± 0.00	eV	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	10.11	eV	NIST Webbook
log10ws	1.46		Crippen Method
logp	2.927		Crippen Method
mcvol	84.390	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3982910&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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