

Phosphonous dichloride, (trichloromethyl)-

Other names: Trichloromethylphosphorous dichloride
Inchi: InChI=1S/CCI5P/c2-1(3,4)7(5)6
InchiKey: RWFGEVVWSNJXRX-UHFFFAOYSA-N
Formula: CCI5P
SMILES: CIP(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 220.25
CAS: 3582-11-4

Physical Properties

Property code	Value	Unit	Source
ie	10.25	eV	NIST Webbook
log10ws	-0.44		Crippen Method
logp	4.104		Crippen Method
mcvol	106.610	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=C3582114&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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<https://www.chemeo.com/cid/46-601-3/Phosphonous-dichloride-trichloromethyl.pdf>

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