

Phosphoramidothioic dichloride, dimethyl-

Other names: Phophonothioamidodichloridate, N,N-dimethyl-Dimethylphosphoramidothioic dichloride
Inchi: InChI=1S/C2H6Cl2NPS/c1-5(2)6(3,4)7/h1-2H3
InchiKey: DWISDTKOMUFVDP-UHFFFAOYSA-N
Formula: C2H6Cl2NPS
SMILES: CN(C)P(=S)(Cl)Cl
Mol. weight [g/mol]: 178.02
CAS: 1498-65-3

Physical Properties

Property code	Value	Unit	Source
ie	8.97 ± 0.04	eV	NIST Webbook
ie	8.97 ± 0.00	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
log10ws	2.21		Crippen Method
logp	2.250		Crippen Method
mcvol	110.310	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C1498653&Units=SI>

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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