

# Methylphosphonothioic acid, S-[2-(diisopropylamino)ethyl] ester

**Other names:** Phosphonothioic acid, methyl, S-(2-(bis-(1-methylethylamino)ethyl) ester)  
**Inchi:** InChI=1S/C9H22NO2PS/c1-8(2)10(9(3)4)6-7-14-13(5,11)12/h8-9H,6-7H2,1-5H3,(H,11,12)  
**InchiKey:** UOXJNGFFPMOZDM-UHFFFAOYSA-N  
**Formula:** C9H22NO2PS  
**SMILES:** CC(C)N(CCSP(C)(=O)O)C(C)C  
**Mol. weight [g/mol]:** 239.31  
**CAS:** 73207-98-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	2.654		Crippen Method
mcvol	196.200	ml/mol	McGowan Method
ripol	2275.00		NIST Webbook
ripol	2275.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C73207984&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**ripol:** Polar retention indices

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