

# Methyldithiophosphonic acid, S-isobutyl, S-(2-diethylaminoethyl) ester

**Inchi:** InChI=1S/C11H26NOPS2/c1-6-12(7-2)8-9-15-14(5,13)16-10-11(3)4/h11H,6-10H2,1-5H3  
**InchiKey:** MSIKPVJRPFOLIK-UHFFFAOYSA-N  
**Formula:** C11H26NOPS2  
**SMILES:** CCN(CC)CCSP(C)(=O)SCC(C)C  
**Mol. weight [g/mol]:** 283.43

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -4.80   |        | Crippen Method |
| logp          | 4.274   |        | Crippen Method |
| mcvol         | 234.860 | ml/mol | McGowan Method |
| rinpol        | 1782.00 |        | NIST Webbook   |
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| rinpol        | 1782.00 |        | NIST Webbook   |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R334780&Units=SI>  
**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>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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