

# o-Ethyl S-nonyl methylphosphonothiolate

**Inchi:** InChI=1S/C12H27O2PS/c1-4-6-7-8-9-10-11-12-16-15(3,13)14-5-2/h4-12H2,1-3H3  
**InchiKey:** AMXPHGZPXNYMOA-UHFFFAOYSA-N  
**Formula:** C12H27O2PS  
**SMILES:** CCCCCCCCSP(C)(=O)OCC  
**Mol. weight [g/mol]:** 266.38  
**CAS:** 13088-89-6

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.09   |        | Crippen Method |
| logp          | 5.330   |        | Crippen Method |
| mcvol         | 228.490 | ml/mol | McGowan Method |
| rinpol        | 1872.00 |        | NIST Webbook   |
| rinpol        | 1872.00 |        | NIST Webbook   |
| rinpol        | 1872.00 |        | NIST Webbook   |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13088896&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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