

# O-(2,4,5-trichlorophenyl) dichloridothiophosphate

**Inchi:** InChI=1S/C6H2Cl5OPS/c7-3-1-5(9)6(2-4(3)8)12-13(10,11)14/h1-2H  
**InchiKey:** NLMYUXLTZXZAJR-UHFFFAOYSA-N  
**Formula:** C6H2Cl5OPS  
**SMILES:** S=P(Cl)(Cl)Oc1cc(Cl)c(Cl)cc1Cl  
**Mol. weight [g/mol]:** 330.38  
**CAS:** 16805-78-0

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -1.79   |        | Crippen Method |
| logp          | 5.728   |        | Crippen Method |
| mcvol         | 175.520 | 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=C16805780&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)

## Legend

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

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