

# O,o-diisopropyl o-(2,4,5-trichlorophenyl) thiophosphate

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C12H16Cl3O3PS/c1-7(2)16-19(20,17-8(3)4)18-12-6-10(14)9(13)5-11(12)15/h5 |
| InchiKey:            | SDIXSYBBSBUHDF-UHFFFAOYSA-N                                                      |
| Formula:             | C12H16Cl3O3PS                                                                    |
| SMILES:              | CC(C)OP(=S)(Oc1cc(Cl)c(Cl)cc1Cl)OC(C)C                                           |
| Mol. weight [g/mol]: | 377.65                                                                           |
| CAS:                 | 64022-00-0                                                                       |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.39   |        | Crippen Method |
| logp          | 6.100   |        | Crippen Method |
| mcvol         | 247.320 | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C64022000&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C64022000&amp;Units=SI</a> |

## Legend

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

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