

Bis(2-chlorophenyl)phosphorochloridate

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|-----------------------------|----------------------------------------------------------------------------------|
| Other names: | Bis(2-chlorophenyl)phosphorochloridate |
| Inchi: | InChI=1S/C12H8Cl3O3P/c13-9-5-1-3-7-11(9)17-19(15,16)18-12-8-4-2-6-10(12)14/h1-8H |
| InchiKey: | ZLSGEMKKBUVQOM-UHFFFAOYSA-N |
| Formula: | C12H8Cl3O3P |
| SMILES: | O=P(Cl)(Oc1ccccc1Cl)Oc1ccccc1Cl |
| Mol. weight [g/mol]: | 337.52 |
| CAS: | 17776-78-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.31 | | Crippen Method |
| logp | 5.798 | | Crippen Method |
| mcvol | 207.210 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C17776782&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | 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 |

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<https://www.chemeo.com/cid/33-553-1/Bis-2-chlorophenyl-phosphorochloridate.pdf>

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