

1-Phenoxysilatrane

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H17NO4Si/c1-2-4-12(5-3-1)17-18-14-9-6-13(7-10-15-18)8-11-16-18/h1-5H |
| InchiKey: | VXZOISSTUSCPNB-UHFFFAOYSA-N |
| Formula: | C12H17NO4Si |
| SMILES: | c1ccc(O[Si]23OCCN(CCO2)CCO3)cc1 |
| Mol. weight [g/mol]: | 267.35 |
| CAS: | 3463-22-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 0.90 | | Crippen Method |
| logp | 0.880 | | Crippen Method |
| rinpol | 2288.00 | | NIST Webbook |
| rinpol | 2288.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3463227&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| rinpol: | Non-polar retention indices |

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<https://www.chemeo.com/cid/29-562-6/1-Phenoxysilatrane.pdf>

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