

Phorate sulfoxide

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| Other names: | Phosphorodithioic acid, O,O-diethyl S-[(ethylsulfinyl)methyl] ester Phorate O-sulfoxide Thimet sulfoxide O,O-Diethyl-S-ethylthionylmethylphosphorodithioate O,O-Diethyl-S-ethylthionylmethyl dithiophosphate O,O-Diethyl S-ethylthionylmethyl thiothionophosphate |
| Inchi: | InChI=1S/C7H17O3PS3/c1-4-9-11(12,10-5-2)13-7-14(8)6-3/h4-7H2,1-3H3 |
| InchiKey: | XRQHTUDGPWMPKX-UHFFFAOYSA-N |
| Formula: | C7H17O3PS3 |
| SMILES: | CCOP(=S)(OCC)SCS(=O)CC |
| Mol. weight [g/mol]: | 276.38 |
| CAS: | 2588-03-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | 1.80 | | Crippen Method |
| logp | 2.743 | | Crippen Method |
| mcvol | 196.610 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2588036&Units=SI |

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/32-140-0/Phorate-sulfoxide.pdf>

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