

Tetraethyl pyrophosphate

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| Other names: | TEPP Diphosphoric acid, tetraethyl ester Pyrophosphoric acid, tetraethyl ester Bis[O,O-diethylphosphoric anhydride] Bladan Ethyl pyrophosphate (Et4P2O7) Nifos Tetraethyl diphosphate Tetrastigmine Tetron Tetron-100 TEP Vapotone Ethyl pyrophosphate, tetra- ENT 18,771 Fosvex Grisol Hepthexamite Killax Kilmite 40 Lethalaire g-52 Lirohex Mortopal Nifost EA 1285 HEPT Hexamite Rcra waste number P111 Killex NSC 14707 |
| Inchi: | InChI=1S/C8H20O7P2/c1-5-11-16(9,12-6-2)15-17(10,13-7-3)14-8-4/h5-8H2,1-4H3 |
| InchiKey: | IDCBOTIENDVCBQ-UHFFFAOYSA-N |
| Formula: | C8H20O7P2 |
| SMILES: | CCOP(=O)(OCC)OP(=O)(OCC)OCC |
| Mol. weight [g/mol]: | 290.19 |
| CAS: | 107-49-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hvap | 82.20 | kJ/mol | NIST Webbook |
| log10ws | -5.14 | | Crippen Method |
| logp | 3.365 | | Crippen Method |
| mcvol | 205.590 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| 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=C107493&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|-----------------|---|
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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