

Tetramethyl methylenediphosphonate

Inchi: InChI=1S/C5H14O6P2/c1-8-12(6,9-2)5-13(7,10-3)11-4/h5H2,1-4H3
InchiKey: XAVFZUKFLWOSOS-UHFFFAOYSA-N
Formula: C5H14O6P2
SMILES: COP(=O)(CP(=O)(OC)OC)OC
Mol. weight [g/mol]: 232.11
CAS: 16001-93-7

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.31 | | Crippen Method |
| logp | 1.916 | | Crippen Method |
| mcvol | 157.450 | 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=C16001937&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/60-211-0/Tetramethyl-methylenediphosphonate.pdf>

Generated by Cheméo on 2024-04-23 15:43:45.577530504 +0000 UTC m=+16176274.498107820.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.