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/ci990307l

Legend

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