

# Phosphonic acid, 1,3-propanediylbis-, tetraethyl ester

**Other names:** Phosphonic acid, trimethylenedi-, tetraethyl ester

Propane-1,3-diphosphonic acid, tetraethyl ester

Tetraethyl propane-1,3-diphosphonate

**Inchi:** InChI=1S/C11H26O6P2/c1-5-14-18(12,15-6-2)10-9-11-19(13,16-7-3)17-8-4/h5-11H2,1-4

**InchiKey:** LJQJJGQRJQSYQN-UHFFFAOYSA-N

**Formula:** C11H26O6P2

**SMILES:** CCOP(=O)(CCCP(=O)(OCC)OCC)OCC

**Mol. weight [g/mol]:** 316.27

**CAS:** 22401-25-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.32		Crippen Method
logp	3.909		Crippen Method
mcvol	241.990	ml/mol	McGowan Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C22401258&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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