

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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=C22401258&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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