1,3-Propanediol, 2,2-dimethyl-, bis(cyclic 2,2-dimethyltrimethylene phosphorothionate

Inchi: InChI=1S/C15H30O6P2S2/c1-13(2,7-16-22(24)18-9-14(3,4)10-19-22)8-17-23(25)20-11-1

InchiKey: YHKBOQACPHKGFG-UHFFFAOYSA-N

Formula: C15H30O6P2S2

SMILES: CC1(C)COP(=S)(OCC(C)(C)COP2(=S)OCC(C)(C)CO2)OC1

Mol. weight [g/mol]: 432.47

CAS: 59609-06-2

Physical Properties

Property code	Value	Unit	Source
log10ws	3.80		Crippen Method
logp	4.641		Crippen Method
mcvol	309.330	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59609062&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume