

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-
InchiKey:	YHKBOQACPHKGFU-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/ci9903071
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

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