Tetraisopropyl methylenediphosphonate

Other names:	tetra-i-Propylmethylenediphosphonate
	Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester
	Methylenediphosphonic acid tetraisopropyl ester
	Phosphonic acid, methylenedi-, tetraisopropyl ester
	tetraisopropyl methylenebisphosphonate
Inchi:	InChI=1S/C13H30O6P2/c1-10(2)16-20(14,17-11(3)4)9-21(15,18-12(5)6)19-13(7)8/h10-1
InchiKey:	ODTQUKVFOLFLIQ-UHFFFAOYSA-N
Formula:	C13H30O6P2
SMILES:	CC(C)OP(=O)(CP(=O)(OC(C)C)OC(C)C)OC(C)C
Mol. weight [g/mol]:	344.32
CAS:	1660-95-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.10		Crippen Method
logp	5.030		Crippen Method
mcvol	270.170	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=C1660953&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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