Ethion oxon

Inchi:	InChI=1S/C9H22O6P2S2/c1-5-12-16(10,13-6-2)18-9-19-17(11,14-7-3)15-8-4/h5-9H2,1-4
InchiKey:	SSEJHKWNPGJOSI-UHFFFAOYSA-N
Formula:	C9H22O6P2S2
SMILES:	CCOP(=O)(OCC)SCSP(=O)(OCC)OCC
Mol. weight [g/mol]:	352.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Crippen Method
logp	4.772		Crippen Method
mcvol	246.510	ml/mol	McGowan Method
rinpol	2149.00		NIST Webbook
rinpol	2149.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R25138&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	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
rinpol:	Non-polar retention indices

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