Fenthoate oxon

Inchi: InChI=1S/C12H17O5PS/c1-4-17-12(13)11(10-8-6-5-7-9-10)19-18(14,15-2)16-3/h5-9,11H
InchiKey: BPHVILLCQZUQEX-UHFFFAOYSA-N
Formula: C12H17O5PS
SMILES: CCOC(=O)C(SP(=O)(OC)OC)c1ccccc1
Mol. weight [g/mol]: 304.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.425		Crippen Method
mcvol	218.040	ml/mol	McGowan Method
rinpol	1925.00		NIST Webbook

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=R543127&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices