

Oxydemeton-methyl M (probably O-analog)

Inchi: InChI=1S/C6H15O5PS/c1-4-13(8)6-5-11-12(7,9-2)10-3/h4-6H2,1-3H3
InchiKey: AJSIYPSFUJBPMF-UHFFFAOYSA-N
Formula: C6H15O5PS
SMILES: CCS(=O)CCOP(=O)(OC)OC
Mol. weight [g/mol]: 230.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	1.173		Crippen Method
mcvol	161.560	ml/mol	McGowan Method
rinpol	1568.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1568.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R494505&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

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