

Piperophos oxon

Inchi: InChI=1S/C14H28NO4PS/c1-4-10-19-20(17,12-18-5-2)21-11-14(16)15-9-7-6-8-13(15)3/h
InchiKey: XQGOTYGTILJJOV-UHFFFAOYSA-N
Formula: C14H28NO4PS
SMILES: CCCOP(=O)(COCC)SCC(=O)N1CCCCC1C
Mol. weight [g/mol]: 337.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.86		Crippen Method
logp	3.734		Crippen Method
mcvol	263.230	ml/mol	McGowan Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R543632&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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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