

O-Isopropyl O-pinacolyl methylthiophosphonate

Inchi: InChI=1S/C10H23O2PS/c1-8(2)11-13(7,14)12-9(3)10(4,5)6/h8-9H,1-7H3
InchiKey: UYXREDLPHWLD AU-UHFFFAOYSA-N
Formula: C10H23O2PS
SMILES: CC(C)OP(C)(=S)OC(C)C(C)(C)C
Mol. weight [g/mol]: 238.33

Physical Properties

Property code	Value	Unit	Source
log10ws	0.57		Crippen Method
logp	3.802		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
rinpol	1347.00		NIST Webbook
rinpol	1347.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R403742&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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