O-Ethyl S-[5-(diisopropylamino)-3-thiapentyl]methylphosp

Inchi: InChI=1S/C13H30NO2PS2/c1-7-16-17(6,15)19-11-10-18-9-8-14(12(2)3)13(4)5/h12-13H,

InchiKey: HUQNCHFSYYONGE-UHFFFAOYSA-N

Formula: C13H30NO2PS2

SMILES: CCOP(C)(=O)SCCSCCN(C(C)C)C(C)C

Mol. weight [g/mol]: 327.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.19		Crippen Method
logp	4.431		Crippen Method
mcvol	268.910	ml/mol	McGowan Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R37361&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.