Phosphorodithioic acid, O,O-dipropyl S-(2-pipecolinocarbonylmethyl) ester

Other names: 1-(Di-N-propoxyphosphinothioylthiomethylcarbonyl-2-methylpiperidine)
Avirosan
C 19490
O,O-Dipropyl S-2-methyl-piperidinocarbonyl-methyl phosphorodithioate
Phosphorodithioic acid, S-[2-(2-methyl-1-piperidinyl)-2-oxoethyl] O,O-dipropyl ester
Piperophos
Rilof

Inchi: InChI=1S/C14H28NO3PS2/c1-4-10-17-19(20,18-11-5-2)21-12-14(16)15-9-7-6-8-13(15)3

InchiKey: UNLYSVIDNRIVFJ-UHFFFAOYSA-N

Formula: C14H28NO3PS2

SMILES: CCCOP(=S)(OCCC)SCC(=O)N1CCCCC1C

Mol. weight [g/mol]: 353.48

CAS: 24151-93-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.15		Aqueous Solubility Prediction Method
log10ws	-4.15		Estimated Solubility Method
logp	4.198		Crippen Method
mcvol	273.710	ml/mol	McGowan Method
rinpol	2471.00		NIST Webbook
rinpol	2469.00		NIST Webbook
rinpol	2464.00		NIST Webbook
rinpol	2466.00		NIST Webbook
rinpol	2486.00		NIST Webbook
rinpol	2466.00		NIST Webbook
rinpol	2464.00		NIST Webbook
rinpol	2466.00		NIST Webbook
rinpol	2486.00		NIST Webbook
ripol	3400.00		NIST Webbook
ripol	3400.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24151937&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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
ripol:	Polar retention indices