Anilofos

Other names:	N-(4-chlorophenyl)-2-dimethoxyphosphinothioylsulfanyl-N-propan-2-ylacetamide
	S-[2-[(4-chlorophenyl)(isopropyl)amino]-2-oxoethyl] O,O-dimethyl dithiophosphate
Inchi:	InChI=1S/C13H19ClNO3PS2/c1-10(2)15(12-7-5-11(14)6-8-12)13(16)9-21-19(20,17-3)18
InchiKey:	NXQDBZGWYSEGFL-UHFFFAOYSA-N
Formula:	C13H19ClNO3PS2
SMILES:	COP(=S)(OC)SCC(=O)N(c1ccc(Cl)cc1)C(C)C
Mol. weight [g/mol]:	367.85
CAS:	64249-01-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Aqueous Solubility Prediction Method
log10ws	-4.43		Estimated Solubility Method
logp	4.332		Crippen Method
mcvol	258.960	ml/mol	McGowan Method
rinpol	2512.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64249010&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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices