Benzoic acid, 2-[[ethoxy[(1-methylethyl)amino]phosphinothioyl]
1-methylethyl ester

Other names:	Amaze
	Amidocid
	Isofenphos
	Isophenphos
	Oftanol
	Pryfon
	Salicylic acid, isopropyl ester, O-ester with O-ethyl isopropylphosphoramidothioate
Inchi:	InChI=1S/C15H24NO4PS/c1-6-18-21(22,16-11(2)3)20-14-10-8-7-9-13(14)15(17)19-12(4
InchiKey:	HOQADATXFBOEGG-UHFFFAOYSA-N
Formula:	C15H24NO4PS
SMILES:	CCOP(=S)(NC(C)C)Oc1ccccc1C(=O)OC(C)C
Mol. weight [g/mol]:	345.39
CAS:	25311-71-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Aqueous Solubility Prediction Method
log10ws	-4.19		Estimated Solubility Method
logp	3.890		Crippen Method
mcvol	264.420	ml/mol	McGowan Method
rinpol	2033.00		NIST Webbook
rinpol	2045.00		NIST Webbook
rinpol	2060.00		NIST Webbook
rinpol	2018.00		NIST Webbook
rinpol	2064.00		NIST Webbook
rinpol	2066.00		NIST Webbook
rinpol	2060.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25311711&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