Fensulfothion

Other names:	B 25141
	BAY 25141
	BAYER 25141
	Bayer S767
	Chemagro 25141
	DMSP
	Daconit
	Dasanit
	ENT 24,945
	O O-Diethyl O-[4-(methylsulphinyl)phenyl phosphorothioate
	O,O-Diaethyl-O-(4-methylsulfinyl-phenyl)-thionophosphat
	O,O-Diaethyl-O-4-methylsulfinyl-phenyl-monothiophosphat
	O,O-Diethyl O-[4-(methylsulfinyl)phenyl] phosphorothioate
	O,O-Diethyl O-[p-(Methylsulfinyl)phenyl] phosphorothioate
	O,O-Diethyl O-p-(methylsulfinyl)phenyl thiophosphate
	OMS 37
	Phenol, p-(methylsulfinyl)-, O-ester with O,O-diethyl phosphorothioate
	Phosphorothioic acid, O,O-diethyl O-[4-(methylsulfinyl)phenyl] ester
	Phosphorothioic acid, O,O-diethyl O-[p-(methylsulfinyl)phenyl] ester
	S 767
	Terracur P
	VUagt 108
	VUagt 96
Inchi:	InChI=1S/C11H17O4PS2/c1-4-13-16(17,14-5-2)15-10-6-8-11(9-7-10)18(3)12/h6-9H,4-5H
InchiKey:	XDNBJTQLKCIJBV-UHFFFAOYSA-N
Formula:	C11H17O4PS2
SMILES:	CCOP(=S)(OCC)Oc1ccc(S(C)=O)cc1
Mol. weight [g/mol]:	308.35
CAS:	115-90-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Aqueous Solubility Prediction Method
log10ws	-2.30		Estimated Solubility Method
logp	3.100		Crippen Method

mcvol	218.730	ml/mol	McGowan Method
rinpol	2265.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115902&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices