Ditalimfos

Other names:	Diethyl phthalimidophosphonothioate
	Ditalimphos
	Dowco 199
	Laptran
	M 2452
	Millie
	O 199
	O,O-Diaethyl-N-phtalimido-thiophosphat
	O,O-Diethyl (1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)phosphonothioate
	O,O-Diethyl phthalimidophosphonothioate
	O,O-Diethyl phthalimidophosphonothionate
	O,O-Diethyl phthalimidothiophosphate
	Ortho 199
	Phosphonothioic acid, (1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-, O,O-diethyl ester
	Phosphonothioic acid, phthalimido-, O,O-diethyl ester
	Phthalimide, N-(diethoxyphosphinothioyl)-
	Plondrel
	RE 199
	SF 101
Inchi:	InChI=1S/C12H14NO4PS/c1-3-16-18(19,17-4-2)13-11(14)9-7-5-6-8-10(9)12(13)15/h5-8H
InchiKey:	MTBZIGHNGSTDJV-UHFFFAOYSA-N
Formula:	C12H14NO4PS
SMILES:	CCOP(=S)(OCC)N1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	299.28
CAS:	5131-24-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Aqueous Solubility Prediction Method
log10ws	-3.35		Estimated Solubility Method
logp	2.580		Crippen Method
mcvol	206.990	ml/mol	McGowan Method
rinpol	2137.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook

tf	357.88 ± 0.20	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5131248&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
tf:	Normal melting (fusion) point