Mefenpyr-diethyl

Other names:	Diethyl (RS)-1-(2,4-dichlorophenyl)-5-methyl-2-pyrazoline-3,5-dicarboxilate Diethyl -1-(2,4-dichlorophenyl)-4,5-dihyfro-5-methyl-1H-pyrazole-3,5-dicarboxilate 1H-Pyrazole-3,5-dicarboxylic acid, 1-(2,4-dichlorophenyl)-4,5-dihydro-5-methyl-, 3,5-diethyl ester 1-(2,4-dichlorophenyl)-4,5-dihydro-5-methyl-1H-pyrazole-3,5-dicarboxylic acid, diethyl ester
Inchi:	InChI=1S/C16H18Cl2N2O4/c1-4-23-14(21)12-9-16(3,15(22)24-5-2)20(19-12)13-7-6-10(1
InchiKey:	OPGCOAPTHCZZIW-UHFFFAOYSA-N
Formula:	C16H18Cl2N2O4
SMILES:	CCOC(=O)C1=NN(c2ccc(Cl)cc2Cl)C(C)(C(=O)OCC)C1
Mol. weight [g/mol]:	373.23
CAS:	135590-91-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	3.444		Crippen Method
mcvol	256.700	ml/mol	McGowan Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C135590919&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