PYRAFLUFEN-ETHYL

Other names:	Acetic acid, 2-[2-chloro-5-[4-chloro-5-(difluoromethoxy)-1-methyl-1H-pyrazol-3-yl]-4-fluorophenoxy]-, ethyl ester
Inchi:	InChI=1S/C15H13Cl2F3N2O4/c1-3-24-11(23)6-25-10-4-7(9(18)5-8(10)16)13-12(17)14(2
InchiKey:	APTZNLHMIGJTEW-UHFFFAOYSA-N
Formula:	C15H13Cl2F3N2O4
SMILES:	CCOC(=O)COc1cc(-c2nn(C)c(OC(F)F)c2Cl)c(F)cc1Cl
Mol. weight [g/mol]:	413.18
CAS:	129630-19-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.00		Crippen Method
logp	4.076		Crippen Method
mcvol	247.920	ml/mol	McGowan Method
rinpol	2355.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C129630199&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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