Flumiclorac-pentyl

Other names:	Acetic acid, 2-[2-chloro-4-fluoro-5-(1,3,4,5,6,7-hexahydro-1,3-dioxo-2H-isoindol-2-yl)phenoxy]-, pentyl ester
Inchi:	InChI=1S/C21H23ClFNO5/c1-2-3-6-9-28-19(25)12-29-18-11-17(16(23)10-15(18)22)24-2
InchiKey:	IRECWLYBCAZIJM-UHFFFAOYSA-N
Formula:	C21H23ClFNO5
SMILES:	CCCCCOC(=O)COc1cc(N2C(=O)C3=C(CCCC3)C2=O)c(F)cc1Cl
Mol. weight [g/mol]:	423.86
CAS:	87546-18-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.60		Crippen Method
logp	4.335		Crippen Method
mcvol	297.410	ml/mol	McGowan Method
rinpol	3080.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87546187&Units=SI
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

Legend

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