Flumioxazin

Inchi: InChI=1S/C19H15FN2O4/c1-2-7-21-15-9-14(13(20)8-16(15)26-10-17(21)23)22-18(24)11
InchiKey: FOUWCSDKDDHKQP-UHFFFAOYSA-N
Formula: C19H15FN2O4
SMILES: C#CCN1C(=O)COc2cc(F)c(N3C(=O)C4=C(CCCC4)C3=O)cc21
Mol. weight [g/mol]: 354.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	1.928		Crippen Method
mcvol	241.640	ml/mol	McGowan Method
rinpol	2950.00		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=R566531&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