difloxacin

Inchi: InChI=1S/C21H19F2N3O3/c1-24-6-8-25(9-7-24)19-11-18-15(10-17(19)23)20(27)16(21(2
InchiKey: NOCJXYPHIIZEHN-UHFFFAOYSA-N
Formula: C21H19F2N3O3
SMILES: CN1CCN(c2cc3c(cc2F)c(=O)c(C(=O)O)cn3-c2ccc(F)cc2)CC1
Mol. weight [g/mol]: 399.39
CAS: 98106-17-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Aqueous Solubility Prediction Method
logp	2.719		Crippen Method
mcvol	275.700	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C98106173&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
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