Ofloxacin

Inchi: InChI=1S/C18H20FN3O4/c1-10-9-26-17-14-11(16(23)12(18(24)25)8-22(10)14)7-13(19)1

InchiKey: GSDSWSVVBLHKDQ-UHFFFAOYSA-N

Formula: C18H20FN3O4

SMILES: CC1COc2c(N3CCN(C)CC3)c(F)cc3c(=O)c(C(=O)O)cn1c23

Mol. weight [g/mol]: 361.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Cheméo Relay (1.0)
logp	1.544		Crippen Method
mcvol	250.430	ml/mol	McGowan Method
tf	526.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Aqueous Solubilities for Ofloxacin, Norfloxacin, Lomefloxacin, Ciprofloxacin, Pefloxacin, and Pipemidic Acid from (293.15 to 323.15) K: https://www.doi.org/10.1021/je7007044

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubility of norfloxacin and ofloxacin in supercritical carbon dioxide: https://www.doi.org/10.1016/j.fluid.2012.06.023

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Determination and Correlation for Solubilities of Ofloxacin, Norfloxacin, Lomefloxacin, Ciprofloxacin, Pefloxacin, and Pipemidic Acid in 1,2-Dichloroethane, Chloroform, Methanol, Acetonitrile, and 1-Octanol from (293.15 to 313.15) K: https://www.doi.org/10.1021/je100116u

Solubility of Ofloxacin in Dichloromethane, Chloroform, Methanol, Acetonitrile, and Water from (293.15 to 333.15) K: https://www.doi.org/10.1021/je900540d

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
tf:	Normal melting (fusion) point

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