pefloxacin

Inchi: InChI=1S/C17H20FN3O3/c1-3-20-10-12(17(23)24)16(22)11-8-13(18)15(9-14(11)20)21-6
InchiKey: FHFYDNQZQSQIAI-UHFFFAOYSA-N
Formula: C17H20FN3O3
SMILES: CCn1cc(C(=O)[O-])c(=O)c2cc(F)c(N3CC[NH+](C)CC3)cc21
Mol. weight [g/mol]: 333.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Cheméo Relay (1.0)
logp	-1.141		Crippen Method
mcvol	241.330	ml/mol	McGowan Method
tf	514.43	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Determination and Correlation for Solubilities of Ofloxacin, Norfloxacin, Lomefloxacin, Ciprofloxacin, Pefloxacin, Lomefloxacin, Norfloxacin, Lomefloxacin, Pefloxacin, and Pipemidic Acid in 1-Octanol from (293.15 to 338.15) K: https://www.doi.org/10.1021/je100116u

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tf: Normal melting (fusion) point

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