

CIPROFLOXACIN

Other names:	1-Cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-qiunolinecarboxylic acid (ciprofloxacin) 1-Cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic acid 1-Cyclopropyl-6-fluoro-4-oxo-7-(1-piperazinyl)-1,4-dihydro-3-quinolinecarboxylic acid 3-Quinolinecarboxylic acid, 1,4-dihydro-1-cyclopropyl-6-fluoro-4-oxo-7-(1-piperazinyl)- 3-Quinolinecarboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)- BAY-o 9867 Bay q 3939 Ciflox Ciprine Cipro IV Ciprobay Ciprofloxacin Ciproxan Ciproxin Ciproxina Velmonit
Inchi:	InChI=1S/C17H18FN3O3/c18-13-7-11-14(8-15(13)20-5-3-19-4-6-20)21(10-1-2-10)9-12(1
InchiKey:	MYSWGUAQZAJ5OK-UHFFFAOYSA-N
Formula:	C17H18FN3O3
SMILES:	O=C(O)c1cn(C2CC2)c2cc(N3CCNCC3)c(F)cc2c1=O
Mol. weight [g/mol]:	331.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Aqueous Solubility Prediction Method
logp	1.583		Crippen Method
mcvol	230.470	ml/mol	McGowan Method
tf	543.00	K	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	64.48	kJ/mol	541.50	NIST Webbook

Sources

Determination and Correlation for Solubilities of Ofloxacin, Norfloxacin, and Ciprofloxacin, Hydroxylation Method: <https://www.doi.org/10.1021/je100116u>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Pefloxacin, and Pipemidic Acid in 1-Octanol from (293.15 to 333.15) K: <http://link.springer.com/article/10.1007/BF02311772>

McGowan Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds: <https://www.doi.org/10.1016/j.jct.2016.10.010>

Solubility Determination and Correlation of Gatifloxacin, Ofloxacin, and Ciprofloxacin, Hydroxylation Method: <https://www.doi.org/10.1021/acs.jced.7b00601>

Aqueous Solubilities for Ofloxacin, Norfloxacin, Ciprofloxacin, Norfloxacin, Ciprofloxacin, and Ciprofloxacin, Hydroxylation Method: <https://www.doi.org/10.1021/je7007044>

Cheméo Relay (1.0): <http://webbook.nist.gov/cgi/cbook.cgi?ID=C85721331&Units=SI>

Legend

hfust: Enthalpy of fusion at a given temperature

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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