

Ciprofloxacin

Other names:	1-Cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic 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:	MYSWGUAQZAJ Sok-UHFFFAOYSA-N
Formula:	C17H18FN3O3
SMILES:	O=C(O)c1cn(C2CC2)c2cc(N3CCNCC3)c(F)cc2c1=O
Mol. weight [g/mol]:	331.34
CAS:	85721-33-1

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

Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds	https://www.doi.org/10.1016/j.jct.2016.10.010
Solubility Determination and Correlation of Gatifloxacin, Enterofloxin and Ciprofloxacin	https://www.doi.org/10.1021/acs.jced.7b00601
Solubilities of Ciprofloxacin, Norfloxacin, Levofloxacin, Ofloxacin, and Norfloxacin in Octanol	https://www.doi.org/10.1021/je100116u
Sublimation and Correlation of Solubilities of Ciprofloxacin, Norfloxacin, Levofloxacin, Ofloxacin, and Norfloxacin in Octanol	https://www.doi.org/10.1021/je7007044
Norfloxacin and Ciprofloxacin in Octanol: Solubility Prediction Method	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Pipemidic Acid from (293.15 to 323.15) K: McGowan Method	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85721331&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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