

1-ETHYL-3-CARBOXY-6-FLUORO-7-(PIPERAZINY

Other names:

1,4-Dihydro-1-ethyl-6-fluoro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic acid
1-Ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic acid
1-Ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic acid
(norfloxacin)
3-Quinolinecarboxylic acid, 1,4-dihydro-1-ethyl-6-fluoro-4-oxo-7-(1-piperazinyl)-
3-Quinolinecarboxylic acid, 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-
AM-715
Baccidal
Barazan
Chibroxin
Chibroxine
Chibroxol
Floxacin
Fulgram
Gonorcin
Lexinor
MK-366
Noflo
Nolicin
Noracin
Noraxin
Norfloxacin
Norocin
Noroxin
Noroxine
Norxacin
Sebercim
Uroxacin
Utinor
Zoroxin
norfloxacin

Inchi: InChI=1S/C16H18FN3O3/c1-2-19-9-11(16(22)23)15(21)10-7-12(17)14(8-13(10)19)20-5-3
InchiKey: OGJPXUAPXNRGGI-UHFFFAOYSA-N
Formula: C16H18FN3O3
SMILES: CCn1cc(C(=O)O)c(=O)c2cc(F)c(N3CCNCC3)cc21
Mol. weight [g/mol]: 319.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Aqueous Solubility Prediction Method
logp	1.268		Crippen Method
mcvol	227.240	ml/mol	McGowan Method
tf	493.50	K	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	32.42	kJ/mol	492.60	NIST Webbook
hfust	32.97	kJ/mol	500.20	NIST Webbook

Sources

Equilibrium study and diversified models of drug Norfloxacin in eight determination and correlation for Solubilities of Ofloxacin, Norfloxacin, Gemifloxacin, Ciprofloxacin, Norfloxacin and Pefloxacin Acid in Aqueous solution (293.15 to 323.15) K.	https://www.doi.org/10.1016/j.fluid.2016.12.012
NIST Webbook:	https://www.doi.org/10.1021/je100116u
McGowan Method:	https://www.doi.org/10.1021/je7007044
Cheméo Relay (1.0):	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Cheméo Relay (1.0, beta):	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70458967&Units=SI
Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds:	http://link.springer.com/article/10.1007/BF02311772
Solubility of norfloxacin and ofloxacin in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.jct.2016.10.010
Crippen Method:	https://www.doi.org/10.1016/j.fluid.2012.06.023
	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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