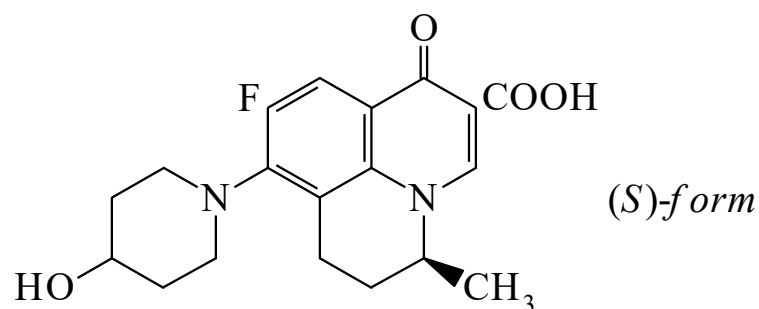




>>Entry Name: Nadifloxacin, BAN, INN

Synonym(s): 9-Fluoro-6,7-dihydro-8-(4-hydroxy-1-piperidiny)-5-methyl-1-oxo-1*H*,5*H*-benzo[*i,j*]quinolizine-2-carboxylic acid, 9Cl. Acuatim. Aquatim. Zinofloxacin. OPC 7251



Related CAS Registry Numbers(s): 81962-84-7 129672-74-8

Molecular Formula: C₁₉H₂₁FN₂O₄

Molecular Weight: 360.384

Accurate Mass: 360.148536

Percentage Composition: C 63.32%; H 5.87%; F 5.27%; N 7.77%; O 17.76%

Biological Use/Importance: Shows strong antibacterial activity against gram positive bacteria. Used for topical treatment of acne

Development Status: Launched 1993 (Japan)

Calculated Log P Data: Log P 0.99 (uncertain value) (calc)

Other Data: Both enantiomers show similar mutagenic props.

>>Variant: (*S*)-form

Molecular Formula: C₁₉H₂₁FN₂O₄

Molecular Weight: 360.384

Accurate Mass: 360.148536

Percentage Composition: C 63.32%; H 5.87%; F 5.27%; N 7.77%; O 17.76%

Physical Description: Cryst. (EtOAc/THF)

Melting Point: Mp 262 dec.°

Optical Rotation: [α]_D²⁰ -314 (c, 1.0 in MeOH) (100% ee)

>>Variant: (±)-form

CAS Registry Number: 124858-35-1

Molecular Formula: C₁₉H₂₁FN₂O₄

Molecular Weight: 360.384

Accurate Mass: 360.148536

Percentage Composition: C 63.32%; H 5.87%; F 5.27%; N 7.77%; O 17.76%

Physical Description: Prisms (EtOH aq.)

Melting Point: Mp 245-247 dec.°

>>Derivative: Me ester

CAS Registry Number: 130539-76-3

Molecular Formula: C₂₀H₂₃FN₂O₄

Molecular Weight: 374.411

Accurate Mass: 374.164186

Percentage Composition: C 64.16%; H 6.19%; F 5.07%; N 7.48%; O 17.09%

Physical Description: Yellow powder (DMF aq.)

Melting Point: Mp 178-182°

References:

- Ishikawa, H. *et al.*, *Chem. Pharm. Bull.*, 1989, **37**, 2103, (*synth, pmr, activity*)
Morita, S. *et al.*, *Chem. Pharm. Bull.*, 1990, **38**, 2027, (*Me ester, synth, cmr, ir*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 183
Takahashi, N. *et al.*, *Arzneim.-Forsch.*, 1994, **44**, 1265, (*mutagenicity*)
Kido, M. *et al.*, *Chem. Pharm. Bull.*, 1994, **42**, 872, (*cryst struct*)
Hashimoto, K. *et al.*, *Chem. Pharm. Bull.*, 1996, **44**, 421; 642, (*synth, cryst struct, abs config*)