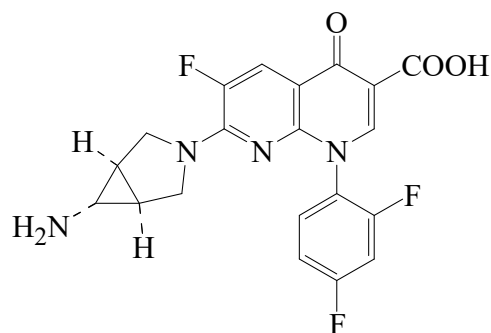




>>Entry Name: Trovafloxacin, INN

Synonym(s): 7-(6-Amino-3-azabicyclo[3.1.0]hex-3-yl)-1-(2,4-difluorophenyl)-6-fluoro-1,4-dihydro-4-oxo-1,8-naphthyridine-3-carboxylic acid, 9Cl. CP 99219



CAS Registry Number: 147059-72-1

Related CAS Registry Numbers(s): 147059-74-3

Molecular Formula: C₂₀H₁₅F₃N₄O₃

Molecular Weight: 416.359

Accurate Mass: 416.109625

Percentage Composition: C 57.70%; H 3.63%; F 13.69%; N 13.46%; O 11.53%

Use/Importance: Antibacterial agent

Development Status: Approved by FDA (1997)

>>Derivative: Hydrochloride

CAS Registry Number: 146961-34-4

Physical Description: Pale yellow solid (MeCN)

Melting Point: Mp 246 dec.°

>>Derivative: Methanesulfonate

Synonym(s): Trovafloxacin mesylate, USAN

CAS Registry Number: 147059-75-4

Solubility: Spar. sol. H₂O (2.3%)

pKa Value: pK_{a1} 8.09 (NH₂); pK_{a2} 5.87 (COOH)

Experimental Log P Data: Log P 0.28 pH 6.5 (exp)

>>Derivative: N-Ac

CAS Registry Number: 175426-02-5

Molecular Formula: C₂₂H₁₇F₃N₄O₄

Molecular Weight: 458.396

Accurate Mass: 458.12019

Percentage Composition: C 57.64%; H 3.74%; F 12.43%; N 12.22%; O 13.96%

Physical Description: Solid (MeOH)

Other Data: Mp >275°

>>Derivative: N-(L-Alanyl-L-alanyl)

References:

- U.S. Pat., 1992, Pfizer, 5 164 402; CA, **119**, 117227w, (synth)
Spangler, S.K. et al., *Antimicrob. Agents Chemother.*, 1994, **38**, 2471, (activity)
Neu, H.C. et al., *Antimicrob. Agents Chemother.*, 1994, **38**, 2615, (activity)
Knapp, J.S. et al., *Antimicrob. Agents Chemother.*, 1995, **39**, 987, (activity)
U.K. Pat., 1995, Pfizer, 2 289 674; CA, **124**, 289514g, (Ac, synth)
Dalvie, D.K. et al., *Drug Metab. Dispos.*, 1996, **24**, 1231-1240; 1997, **25**, 423-427, (metab)
Teng, R. et al., *J. Chromatogr., B: Biomed. Appl.*, 1996, **675**, 53-59, (hplc)
Haria, M. et al., *Drugs*, 1997, **54**, 435-445, (rev)
Brighty, K.E. et al., *J. Antimicrob. Chemother., Suppl. B*, 1997, **39**, 1-14, (rev)