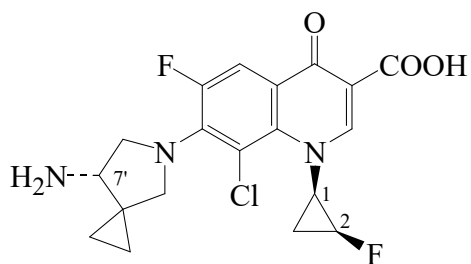




>>Entry Name: Sitafloracin, INN

Synonym(s): 7-(7-Amino-5-azaspiro[2.4]hept-5-yl)-8-chloro-6-fluoro-1-(2-fluorocyclopropyl)-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid, 9Cl. DU 6859



(1*R*,2*S*,7'*S*)-form

Molecular Formula: C₁₉H₁₈ClF₂N₃O₃

Molecular Weight: 409.819

Accurate Mass: 409.100475

Percentage Composition: C 55.69%; H 4.43%; Cl 8.65%; F 9.27%; N 10.25%; O 11.71%

Biological Use/Importance: Antibacterial agent

>>Variant: (1*R*,2*S*,7'*S*)-form

CAS Registry Number: 127254-12-0

Molecular Formula: C₁₉H₁₈ClF₂N₃O₃

Molecular Weight: 409.819

Accurate Mass: 409.100475

Percentage Composition: C 55.69%; H 4.43%; Cl 8.65%; F 9.27%; N 10.25%; O 11.71%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 225° (dec.)

Optical Rotation: [α]_D -199.9 (1*M* NaOH)

Other Data: Pharmacol. active isomer

>>Variant: (1*R*,2*S*,7'*R*)-form

CAS Registry Number: 127254-10-8

Molecular Formula: C₁₉H₁₈ClF₂N₃O₃

Molecular Weight: 409.819

Accurate Mass: 409.100475

Percentage Composition: C 55.69%; H 4.43%; Cl 8.65%; F 9.27%; N 10.25%; O 11.71%

Melting Point: Mp 121-127°

Optical Rotation: [α]_D -21.2 (1*M* NaOH)

>>Variant: (1*S*,2*R*,7'*R*)-form

CAS Registry Number: 127199-06-8

Molecular Formula: C₁₉H₁₈ClF₂N₃O₃

Molecular Weight: 409.819

Accurate Mass: 409.100475

Percentage Composition: C 55.69%; H 4.43%; Cl 8.65%; F 9.27%; N 10.25%; O 11.71%

Melting Point: Mp 126-160° (dec.)

Optical Rotation: [α]_D +186.8 (1*M* NaOH)

>>Variant: (1*S*,2*R*,7'*S*)-form

CAS Registry Number: 127254-11-9

Molecular Formula: C₁₉H₁₈ClF₂N₃O₃

Molecular Weight: 409.819

Accurate Mass: 409.100475

Percentage Composition: C 55.69%; H 4.43%; Cl 8.65%; F 9.27%; N 10.25%; O 11.71%

Melting Point: Mp 123-128°

Optical Rotation: [α]_D +21.5 (1*M* NaOH)

References:

Eur. Pat., 1989, *Daiichi Seiyaku*, 341 493; *CA*, **113**, 40473q, (*synth, pharmacol*)

Sato, K. *et al.*, *Antimicrob. Agents Chemother.*, 1992, **36**, 1491-1498, (*activity*)

Kimura, Y. *et al.*, *J. Med. Chem.*, 1994, **37**, 3344-3352, (*synth, pmr, pharmacol*)

Nakashima, M. *et al.*, *Antimicrob. Agents Chemother.*, 1995, **39**, 170-174, (*activity*)