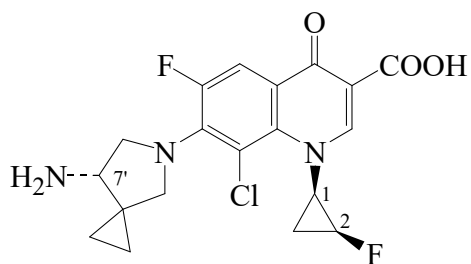




>>Entry Name: Sitafloracin, INN

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:** C<sub>19</sub>H<sub>18</sub>ClF<sub>2</sub>N<sub>3</sub>O<sub>3</sub>

**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:** C<sub>19</sub>H<sub>18</sub>ClF<sub>2</sub>N<sub>3</sub>O<sub>3</sub>

**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:** [ $\alpha$ ]<sub>D</sub> -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:** C<sub>19</sub>H<sub>18</sub>ClF<sub>2</sub>N<sub>3</sub>O<sub>3</sub>

**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:** [ $\alpha$ ]<sub>D</sub> -21.2 (1*M* NaOH)

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

**CAS Registry Number:** 127199-06-8

**Molecular Formula:** C<sub>19</sub>H<sub>18</sub>ClF<sub>2</sub>N<sub>3</sub>O<sub>3</sub>

**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:** [ $\alpha$ ]<sub>D</sub> +186.8 (1*M* NaOH)

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

**CAS Registry Number:** 127254-11-9

**Molecular Formula:** C<sub>19</sub>H<sub>18</sub>ClF<sub>2</sub>N<sub>3</sub>O<sub>3</sub>

**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:** [ $\alpha$ ]<sub>D</sub> +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*)