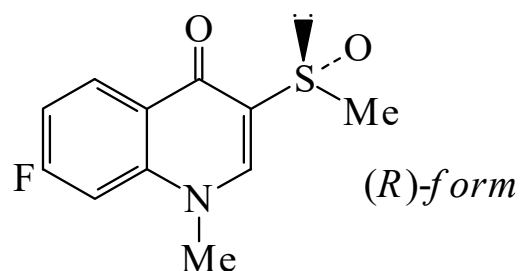




>>Entry Name: Flosequinan, BAN, INN, USAN

Synonym(s): 7-Fluoro-1-methyl-3-(methylsulfinyl)-4(1*H*)-quinolinone, 9Cl. Manoplax. BTS 49465



CAS Registry Number: 76568-02-0

Molecular Formula: C<sub>11</sub>H<sub>10</sub>FNO<sub>2</sub>S

Molecular Weight: 239.27

Accurate Mass: 239.041627

Percentage Composition: C 55.22%; H 4.21%; F 7.94%; N 5.85%; O 13.37%; S 13.40%

Use/Importance: Vasodilator, antihypertensive agent, cardiostimulant

Development Status: Withdrawn from clinical use in the UK (1993)

Calculated Log P Data: Log P -0.35 (calc)

>>Variant: (*R*)-form

CAS Registry Number: 154504-93-5

Molecular Formula: C<sub>11</sub>H<sub>10</sub>FNO<sub>2</sub>S

Molecular Weight: 239.27

Accurate Mass: 239.041627

Percentage Composition: C 55.22%; H 4.21%; F 7.94%; N 5.85%; O 13.37%; S 13.40%

Optical Rotation:  $[\alpha]_D^{25} +405$  (c, 1 in CHCl<sub>3</sub>) (99.6% ee)

>>Variant: (*S*)-form

CAS Registry Number: 154504-94-6

Molecular Formula: C<sub>11</sub>H<sub>10</sub>FNO<sub>2</sub>S

Molecular Weight: 239.27

Accurate Mass: 239.041627

Percentage Composition: C 55.22%; H 4.21%; F 7.94%; N 5.85%; O 13.37%; S 13.40%

Physical Description: Prisms

Melting Point: Mp 258-258.5 dec.°

Optical Rotation:  $[\alpha]_D^{25} -393$  (c, 1 in CHCl<sub>3</sub>) (98.5% ee)

>>Variant: (±)-form

Molecular Formula: C<sub>11</sub>H<sub>10</sub>FNO<sub>2</sub>S

Molecular Weight: 239.27

Accurate Mass: 239.041627

Percentage Composition: C 55.22%; H 4.21%; F 7.94%; N 5.85%; O 13.37%; S 13.40%

Physical Description: Cryst.

Melting Point: Mp 226-228°

>>Derivative: S-Oxide

Synonym(s): Flosequinoxan

Molecular Formula: C<sub>11</sub>H<sub>10</sub>FNO<sub>3</sub>S

Molecular Weight: 255.269

Accurate Mass: 255.036542

Percentage Composition: C 51.76%; H 3.95%; F 7.44%; N 5.49%; O 18.80%; S 12.56%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 231-236°

References: