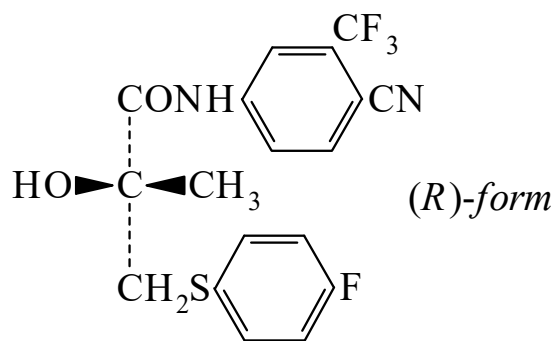




>>Entry Name: *N*-[4-Cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)thio]-2-hydroxy-2-methylpropanamide, 9Cl



**CAS Registry Number:** 90356-78-8

**Molecular Formula:** C<sub>18</sub>H<sub>14</sub>F<sub>4</sub>N<sub>2</sub>O<sub>2</sub>S

**Molecular Weight:** 398.38

**Accurate Mass:** 398.07121

**Percentage Composition:** C 54.27%; H 3.54%; F 19.08%; N 7.03%; O 8.03%; S 8.05%

**Other Data:** Synthetic precursor of Bicalutamide [NDR64-I](#)

>>Variant: (*R*)-form

**CAS Registry Number:** 90357-17-8

**Molecular Formula:** C<sub>18</sub>H<sub>14</sub>F<sub>4</sub>N<sub>2</sub>O<sub>2</sub>S

**Molecular Weight:** 398.38

**Accurate Mass:** 398.07121

**Percentage Composition:** C 54.27%; H 3.54%; F 19.08%; N 7.03%; O 8.03%; S 8.05%

**Melting Point:** Mp 94-96°

**Optical Rotation:**  $[\alpha]_{\text{D}}^{24} -3.06$  (c, 1.01 in MeOH)

>>Derivative: *S,S*-Dioxide

*see* Bicalutamide, [NDR64-I](#)

>>Variant: (*S*)-form

**CAS Registry Number:** 90357-18-9

**Molecular Formula:** C<sub>18</sub>H<sub>14</sub>F<sub>4</sub>N<sub>2</sub>O<sub>2</sub>S

**Molecular Weight:** 398.38

**Accurate Mass:** 398.07121

**Percentage Composition:** C 54.27%; H 3.54%; F 19.08%; N 7.03%; O 8.03%; S 8.05%

**Physical Description:** Cryst. (toluene/petrol)

**Melting Point:** Mp 94.5-96.5°

**Optical Rotation:**  $[\alpha]_{\text{D}}^{24} +2.32$  (MeOH)

#### References:

Tucker, H. *et al.*, *J. Med. Chem.*, 1988, **31**, 885; 954, (*synth*)