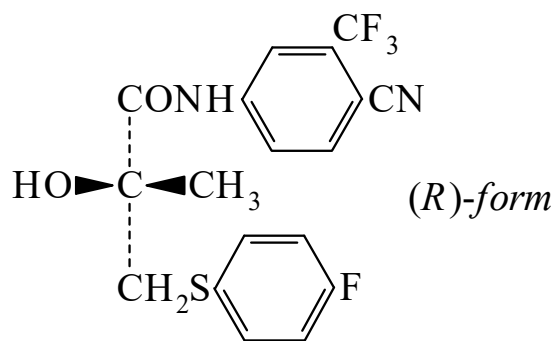




>>Entry Name: *N*-[4-Cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)thio]-2-hydroxy-2-methylpropanamide, 9Cl



CAS Registry Number: 90356-78-8

Molecular Formula: C₁₈H₁₄F₄N₂O₂S

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: C₁₈H₁₄F₄N₂O₂S

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: [α]_D²⁴ -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: C₁₈H₁₄F₄N₂O₂S

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: [α]_D²⁴ +2.32 (MeOH)

References:

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