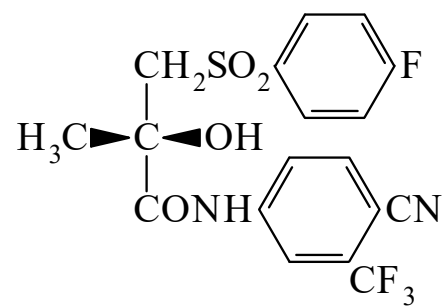




>>Entry Name: Bicalutamide, BAN, INN, USAN

Synonym(s): *N*-[4-Cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanamide. Casodex. ICI 176334



CAS Registry Number: 90357-06-5

Related CAS Registry Numbers(s): 113299-38-0 151262-58-7

Molecular Formula: C₁₈H₁₄F₄N₂O₄S

Molecular Weight: 430.379

Accurate Mass: 430.06104

Percentage Composition: C 50.23%; H 3.28%; F 17.66%; N 6.51%; O 14.87%; S 7.45%

Use/Importance: Antiandrogen investigated for the treatment of advanced prostate cancer

Development Status: Launched 1995 (UK)

Calculated Log P Data: Log P 2.68 (calc)

>>Variant: (*R*)-form

CAS Registry Number: 113299-40-4

Molecular Formula: C₁₈H₁₄F₄N₂O₄S

Molecular Weight: 430.379

Accurate Mass: 430.06104

Percentage Composition: C 50.23%; H 3.28%; F 17.66%; N 6.51%; O 14.87%; S 7.45%

Melting Point: Mp 179-180°

Optical Rotation: $[\alpha]_{\text{D}}^{24} -80.04$ (c, 1.02 in MeOH)

Other Data: Pharmacol. active isomer

>>Variant: (±)-form

Molecular Formula: C₁₈H₁₄F₄N₂O₄S

Molecular Weight: 430.379

Accurate Mass: 430.06104

Percentage Composition: C 50.23%; H 3.28%; F 17.66%; N 6.51%; O 14.87%; S 7.45%

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 191-193°

References:

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