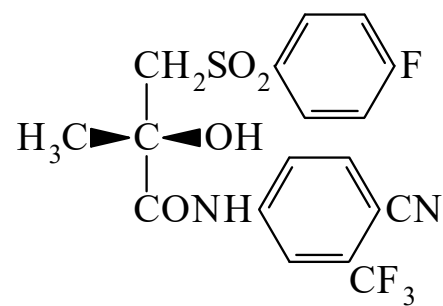




>>Entry Name: Bicalutamide, BAN, INN, USAN

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: ($\pm$)-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:

- Eur. Pat.*, 1984, *ICI*, 100 172; *CA*, **101**, 54739v, (*synth*)
Tucker, H. *et al.*, *J. Med. Chem.*, 1988, **31**, 885; 954, (*synth, resoln, pharmacol*)
Furr, B.J.A., *Prog. Clin. Biol. Res.*, 1988, **260**, 13, (*rev*)
Cockshott, I.D. *et al.*, *Xenobiotica*, 1991, **21**, 1347, (*pharmacol*)
Blackledge, G., *Cancer (Philadelphia), Suppl.*, 1993, **72**, 3830, (*rev*)
Boyle, G.W. *et al.*, *Xenobiotica*, 1993, **23**, 781; 1241, (*metab*)
Furr, B.J.A., *Ann. N.Y. Acad. Sci.*, 1995, **761**, 79, (*rev*)
Schellhammer, P., *Expert Opin. Invest. Drugs*, 1999, **8**, 849-860