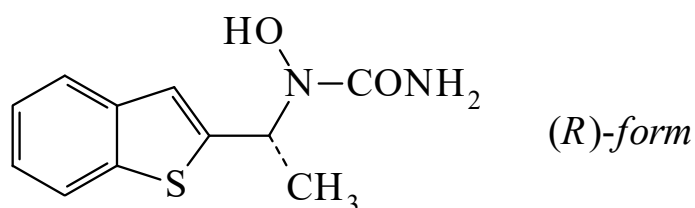




>>Entry Name: Zileuton, BAN, INN, USAN

Synonym(s): *N*-(1-Benzo[*b*]thien-2-ylethyl)-*N*-hydroxyurea, 9CI. Abbott 64077. ABT 077



CAS Registry Number: 111406-87-2

Related CAS Registry Numbers(s): 118569-21-4 143200-94-6 154003-29-9

Molecular Formula: C₁₁H₁₂N₂O₂S

Molecular Weight: 236.294

Accurate Mass: 236.061948

Percentage Composition: C 55.91%; H 5.12%; N 11.86%; O 13.54%; S 13.57%

Biological Use/Importance: 5-Lipoxygenase inhibitor. Antiallergic, antiinflammatory agent. Potential antiasthmatic agent. Investigated for treatment of irritable bowel disease

Development Status: Approved by FDA (1996)

Calculated Log P Data: Log P 2.64 (uncertain value) (calc)

>>Variant: (*R*)-form

CAS Registry Number: 142606-21-1

Molecular Formula: C₁₁H₁₂N₂O₂S

Molecular Weight: 236.294

Accurate Mass: 236.061948

Percentage Composition: C 55.91%; H 5.12%; N 11.86%; O 13.54%; S 13.57%

Melting Point: Mp 148-149°

Optical Rotation: [α]_D +50.3 (c, 0.35 in MeOH). [α]_D²⁴ +47 (c, 1 in MeOH)

>>Variant: (±)-form

CAS Registry Number: 154003-29-9

Molecular Formula: C₁₁H₁₂N₂O₂S

Molecular Weight: 236.294

Accurate Mass: 236.061948

Percentage Composition: C 55.91%; H 5.12%; N 11.86%; O 13.54%; S 13.57%

Physical Description: Solid (EtOAc/hexane)

Melting Point: Mp 158-160°

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