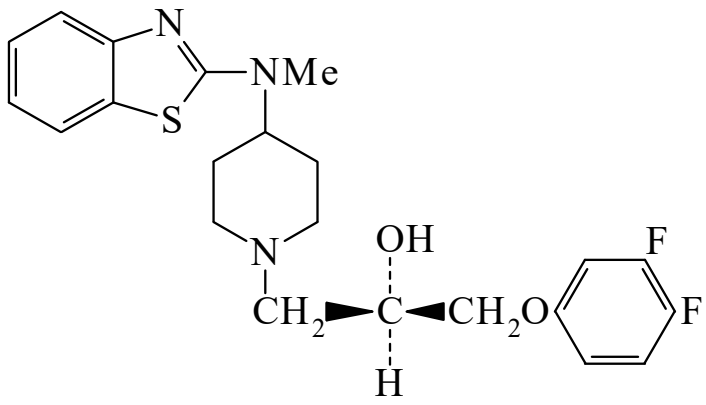
>>**Entry Name: Lubeluzole,** BAN, INN

Synonym(s): 4-(2-Benzothiazolylmethylamino)-α-[(3,4-difluorophenoxy)methyl]-1-piperidineethanol, 9CI. R 87926



(*S*)-*form*

Molecular Formula: $C_{22}H_{25}F_2N_3O_2S$
Molecular Weight: 433.521
Accurate Mass: 433.163553
Percentage Composition: C 60.95%; H 5.81%; F 8.76%; N 9.69%; O 7.38%; S 7.40%
Use/Importance: Neuroprotective and antihypoxic agent. Used in the treatment of cerebral ischaemia
Development Status: In Phase II clinical trials (1996)
Other Data: Analogue of Sabeluzole BST71-R
Hazard & Toxicity: Exp. cardiovascular effects

>>**Variant:** (*S*)-form

CAS Registry Number: 144665-07-6
Molecular Formula: $C_{22}H_{25}F_2N_3O_2S$
Molecular Weight: 433.521
Accurate Mass: 433.163553
Percentage Composition: C 60.95%; H 5.81%; F 8.76%; N 9.69%; O 7.38%; S 7.40%
Physical Description: Cryst. (diisopropyl ether)
Melting Point: Mp 65.8°
Optical Rotation: $[\alpha]_D^{20}$+4.38 (c, 1 in MeOH)
Other Data: Pharmacol. active isomer

>>**Derivative:** Hydrochloride (1:2)

CAS Registry Number: 144665-09-8
Melting Point: Mp 148.7°
Optical Rotation: $[\alpha]_D^{20}$–9.01 (c, 1 in MeOH)

>>**Derivative:** Hydrobromide (1:2)

CAS Registry Number: 144730-87-0
Melting Point: Mp 213.7°

>>**Variant:** (±)-form

CAS Registry Number: 144574-26-5
Molecular Formula: $C_{22}H_{25}F_2N_3O_2S$
Molecular Weight: 433.521
Accurate Mass: 433.163553
Percentage Composition: C 60.95%; H 5.81%; F 8.76%; N 9.69%; O 7.38%; S 7.40%
Melting Point: Mp 86.4°

>>**Derivative:** Hydrochloride (1:2)

CAS Registry Number: 144574-25-4
Melting Point: Mp 211.8°

References:

Eur. Pat., 1992, *Janssen*, 501 552; *CA*, **118**, 80927a, *(synth, pharmacol)*
Peeters, O.M. *et al.*, *Acta Cryst. C*, 1995, **51**, 2129, *(cryst struct)*
De Ryck, M. *et al.*, *J. Pharmacol. Exp. Ther.*, 1996, **279**, 748; 759, *(pharmacol)*
Diener, H.C. *et al.*, *Stroke (Dallas)*, 1996, **27**, 76, *(clin trial)*
Sugiyama, A. *et al.*, *Toxicol. Appl. Pharmacol.*, 1996, **139**, 109, *(tox)*
Maiese, K. *et al.*, *J. Neurochem.*, 1997, **68**, 710, *(pharmacol)*

https://www.baizuoyan.com - CopyRight ©baizuoyan