

PRODUCT INFORMATION



Batefenterol

Item No. 21793

CAS Registry No.: 743461-65-6
Formal Name: N-[1,1'-biphenyl]-2-yl-carbamic acid, 1-[3-[[2-chloro-4-[[[(2R)-2-(1,2-dihydro-8-hydroxy-2-oxo-5-quinoliny)-2-hydroxyethyl]amino]methyl]-5-methoxyphenyl]amino]-3-oxopropyl]-4-piperidinyl ester

Synonyms: GSK961081, TD-5959

MF: C₄₀H₄₂ClN₅O₇

FW: 740.2

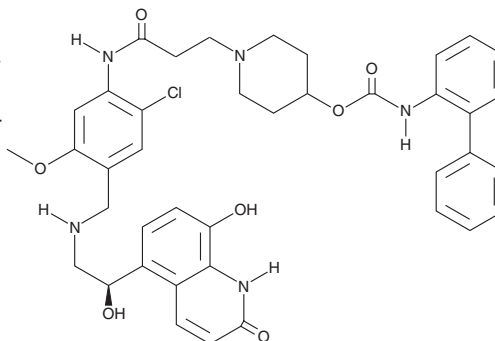
Purity: ≥98%

UV/Vis.: λ_{max}: 254, 293 nm

Supplied as: A crystalline solid

Storage: -20°C

Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Batefenterol is supplied as a crystalline solid. A stock solution may be made by dissolving the batefenterol in the solvent of choice, which should be purged with an inert gas. Batefenterol is soluble in organic solvents such as DMSO and dimethyl formamide (DMF). The solubility of batefenterol in these solvents is approximately 0.5 and 1 mg/ml, respectively.

Batefenterol is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, batefenterol should first be dissolved in DMF and then diluted with the aqueous buffer of choice. Batefenterol has a solubility of approximately 0.25 mg/ml in a 1:3 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Batefenterol is a muscarinic antagonist and β₂-adrenergic receptor (β₂-AR) agonist (K_s = 1.4, 1.3, and 3.7 nM, for hM₂, hM₃, and hβ₂-AR, respectively in a radioligand binding assay).^{1,2} Batefenterol exhibits potent hβ₂-AR agonist activity (EC₅₀ = 0.29 nM) with 440- and 320-fold functional selectivity over hβ₁- and hβ₃-ARs, respectively.¹ Batefenterol induces smooth muscle relaxation (EC₅₀ = 11 nM) in isolated guinea pig tracheal tissue and inhibits bronchoconstrictor response in a guinea pig bronchoprotection assay (ED₅₀ = 6.4 μg/ml).¹ Formulations containing batefenterol are in clinical trials to treat chronic obstructive pulmonary disease (COPD).³

References

1. Hedge, S.S., Hughes, A.D., Chen, Y., et al. *J. Pharmacol. Exp. Ther.* **351**(1), 190-199 (2014).
2. Hughes, A.D., Chen, Y., Hegde, S.S., et al. *J. Med. Chem.* **58**(6), 2609-2622 (2015).
3. Wielders, P.L.M.L., Ludwig-Sengpiel, A., Locantore, N., et al. *Eur. Respir.* **42**(4), 972-981 (2013).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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