
Product Data Sheet

Product Name: Tiotropium Bromide hydrate

Cat. No.: GC13134

Chemical Properties

Cas. No. 139404-48-1

Chemical Name (1R,2R,4S,5S,7s)-7-(2-hydroxy-2,2-di(thiophen-2-yl)acetoxy)-9,9-dimethyl-3-oxa-9-azatricyclo[3.3.1.0^{2,4}]nonan-9-ium bromide hydrate

SMILES
O=C(C(C1=C([H])C([H])=C([H])S1)(C2=C([H])C([H])=C([H])S2)O[H])O[C@@]3([H])C([H])([H])[C@]4([H])[N+](C([H])([H])[H])(C([H])([H])[H])[C@@](C3([H])[H])([H])[C@@]5([H])O[C@@]45[H].[H]O[H].[Br-]

Formula	C ₁₉ H ₂₂ NO ₄ S ₂ .Br.xH ₂ O	M.Wt	490.43
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Solubility	DMSO : 8mg/mL	Storage	Store at -20°C
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General tips For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.

Structure **Background**

Tiotropium Bromide hydrate is an anticholinergic and bronchodilator and a muscarinic receptor antagonist. Target: mAChRTiotropium bromide (Ba 679 BR) is a novel potent and long-lasting muscarinic antagonist that has been developed for the treatment of chronic obstructive airways disease (COPD). Binding studies with [³H]tiotropium bromide in human lung have confirmed that this is a potent muscarinic antagonist with equal affinity for M₁-, M₂- and M₃-receptors and is approximately 10-fold more potent than ipratropium bromide. In vitro tiotropium bromide has a potent inhibitory effect against cholinergic nerve-induced contraction of guinea-pig and human airways, that has a slower onset than atropine or ipratropium bromide. tiotropium bromide dissociates slowly from M₃-receptors (on airway smooth muscle) but rapidly from M₂ autoreceptors (on cholinergic nerve terminals) [1]. Tiotropium bromide is a quaternary ammonium

Caution: Product has not been fully validated for medical applications. For research use only.

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derivative that binds to muscarinic receptors. However, although tiotropium binds with high affinity to muscarinic receptors of M1-, M2- and M3-subtypes, it dissociates very slowly from M1- and M3-receptors but more rapidly from M2-receptors, thereby giving it a unique kinetic selectivity [2].

References:

- [1]. Barnes, P.J., et al., Tiotropium bromide (Ba 679 BR), a novel long-acting muscarinic antagonist for the treatment of obstructive airways disease. *Life Sci*, 1995. 56(11-12): p. 853-9.
- [2]. Hansel, T.T. and P.J. Barnes, Tiotropium bromide: a novel once-daily anticholinergic bronchodilator for the treatment of COPD. *Drugs Today (Barc)*, 2002. 38(9): p. 585-600.

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