Product Data Sheet

Product Name: Epelsiban (GSK 557296)
Cat. No.: GC30594

Chemical Properties

Cas. No.	872599-83-2		
SMILES	O=C(N1CCOCC1)[C@@H](C2=C(N=C(C)C=C2)C)N3[C@](C(N[C@H](C4CC5=CC=CC=C5C4)C3=O)=O)([H])[C@@H](C)CC		
Formula	$C_{30}H_{38}N_4O_4$	M.Wt	518.65
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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	Epelsiban (GSK 557296)		

Background

Epelsiban (GSK 557296) is a potent, selective and orally bioavailable oxytocin receptor antagonist, with a pKi of 9.9 for human oxytocin receptor.

Epelsiban is a potent oxytocin receptor, with a pKi of 9.9 for human oxytocin receptor, >31000-fold selectivity over all three human vasopressin receptors hV1aR (pKi,

Epelsiban shows an IC50 of 192 nM for oxytocin receptor in rats. Epelsiban has low levels of intrinsic clearance against the microsomes of rat, dog, and cynomolgus monkey, good bioavailability (55%), but is negative in the genotoxicity screens with a satisfactory oral safety profile in female rats[1].

[1]. Borthwick AD, et al. Pyridyl-2,5-diketopiperazines as potent, selective, and orally bioavailable oxytocin antagonists: synthesis, pharmacokinetics, and in vivo potency. J Med Chem. 2012 Jan 26;55(2):783-96.

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