



Formula: C<sub>22</sub>H<sub>35</sub>NO<sub>2</sub>

MW: 345.53

CAS: 6879-74-9

TNP NUMBER: TNP00617

MDL NUMBER: MFCD00274559

IUPAC: 8-[(1E)-2-((2S,6R)-1,6-dimethyl(2-piperidyl))vinyl](3S,6S,9S,1R,7R,8R)-6-methyl-5-oxatricyclo[7.4.0.0]tridecan-4-one

Smiles:

C1C[C@@H]2([C@H]([C@@H]3[C@H](C[C@H]2CC1)C(=O)O[C@H]3C)C=C[C@H]1N([C@@H](CCC1)C)C)

Himbacine is an alkaloid isolated from *Galbulimima baccata*. It is a potent muscarinic M<sub>2</sub>/M<sub>4</sub> receptor antagonist<sup>1,2</sup>

REFERENCE: Doller, D., et al., Design, synthesis, and structure-activity relationship studies of himbacine derived muscarinic receptor antagonists. *Bioorg. Med. Chem. Lett.* 9, 901-906, (1999) abstract  
Sagrada, A., et al., Himbacine discriminates between putative muscarinic M<sub>1</sub> receptor-mediated responses. *Life Sci.* 54, PL305-PL310, (1994) abstract  
Miller, J.H., et al., Binding and functional selectivity of himbacine for cloned and neuronal muscarinic receptors. *J. Pharmacol. Exp. Ther.* 263, 663-667, (1992) abstract  
Dorje, F., et al., Antagonist binding profiles of five cloned human muscarinic receptor subtypes. *J. Pharmacol. Exp. Ther.* 256, 727-733, (1991) abstract

SOURCE: Himbacine is an alkaloid isolated from *Galbulimima baccata*.

ACCEPTORS: 2

DONORS: 0

ROTATION BONDS: 0

N+O: 3

Chiral Centers: 8

LogP: 7.32

LogS: -5.92

LIPINSKI: 3

