

Product Information

Atracurium besylate, Purity ≥98%

Cat. No.: X24-09-YM1134

Size: 10 mg; 25 mg; 50 mg; 100 mg

CAS Number: 64228-81-5

Compound CID: 47320

Synonym: 64228-81-5; atracurium besilate; Tracrium; Atracurium Dibesylate;

Atracurium (besylate); Besilate d'atracurium; Besilato de atracurio; Benzenesulfonate;

5-[3-[1-[(3

,4-dimethoxyphenyl

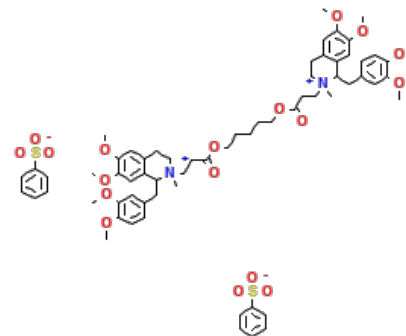
)methyl]-6,7-dimethoxy-2-methyl-3,4-di

hydro-1*H*-isoquinolin-2-ium-2-yl]propanoyloxy]pentyl

3-[1-[(3,4-di

methoxyphenyl)methyl]-

6,7-dimethoxy-2-methyl-3,4-dihydro-1*H*-isoquinolin-2-ium-2-yl]propanoate



This product is for research use only and is not intended for diagnostic use.

Product Information

Description	Atracurium besylate, soluble in DMSO, water, and ethanol, is a neuromuscular blocking agent. The molecular weight of the compound is 1243.48, and its molecular formula is $C_{53}H_{72}N_2O_{12} \cdot 2(C_6H_5O_3S)$.
Molecular Weight	1243.48
Molecular Formula	$C_{53}H_{72}N_2O_{12} \cdot 2(C_6H_5O_3S)$
IUPAC Name	Benzenesulfonate; 5-[3-[1-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxy-2-methyl-3,4-dihydro-1 <i>H</i> -isoquinolin-2-ium-2-yl]propanoyloxy]pentyl 3-[1-[(3,4-dimethoxyphenyl)methyl]-6,7-dimethoxy-2-methyl-3,4-dihydro-1 <i>H</i> -isoquinolin-2-ium-2-yl]propanoate
InChI	InChI=1S/C53H72N2O12.2C6H6O3S/c1-54(22-18-38-32-48(62-7)50(64-9)34-40(38)42(54)28-36-14-16-44(58-3)46(30-36)60-5)24-20-52(56)66-26-12-11-13-27-67-53(57)21-25-55(2)23-19-39-33-49(63-8)51(65-10)35-41(39)43(55)29-37-15-17-45(59-4)47(31-37)61-6;2*7-10(8,9)6-4-2-1-3-5-6/h14-17,30-35,42-43H,11-13,18-29H2,1-10H3;2*1-5H,(H,7,8,9)/q+2;;/p-2

InChI Key	XXZSQOVSEBAPGS-UHFFFAOYSA-L
Canonical SMILES	<chem>C[N+]1(CCC2=CC(=C(C=C2C1CC3=CC(=C(C=C3)OC)OC)OC)OC)CCC(=O)OCCCCCOC(=O)CC[N+]4(CCC5=CC(=C(C=C5C4CC6=CC(=C(C=C6)OC)OC)OC)OC)C.C1=CC=C(C=C1)S(=O)(=O)[O-].C1=CC=C(C=C1)S(=O)(=O)[O-]</chem>
Isomeric SMILES	<chem>C[C@]12C=CC3=C4CCC(=O)C=C4CC[C@H]3[C@@@H]1CC[C@]2(CC=C)O</chem>
Form	Lyophilized powder
Purity	≥98%
Impurities	Free from inappropriate visible particulates, foreign matter, discoloration, or other defects.
Solubility	<i>In vitro</i> : DMSO: 96 mg/mL (77.19 mM); Water (warmed): 32 mg/mL (25.73 mM); Ethanol: 96 mg/mL (77.19 mM)
Identity	Confirmed by NMR/HPLC/MS.
Stability	In its lyophilized form, the chemical remains stable for 36 months.
Quality Level	Research grade
Applications	Atracurium besylate plays a key role in inhibiting nicotinic acetylcholine receptors at the neuromuscular junction, preventing muscle contraction.
Storage	Store at -20°C, and keep desiccated.
