



Product Information

6-Mono-O-(*p*-toluenesulfonyl)- β -cyclodextrin

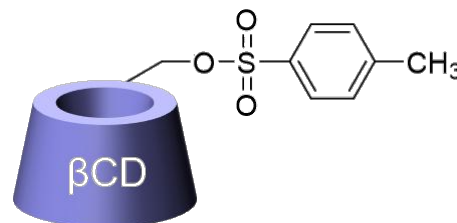
Cat. No.: X23-11-YM127

Size: 1 g; 2 g; 5 g; 10 g

CAS Number: 67217-55-4

Synonym: 6-Monotosyl-BCD, MoTsBCD

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



Product Information

Molecular Weight	1289.2
Molecular Formula	C ₄₉ H ₇₆ O ₃₇ S
IUPAC Name	[(1 <i>S</i> ,3 <i>R</i> ,5 <i>R</i> ,6 <i>S</i> ,8 <i>R</i> ,10 <i>R</i> ,11 <i>S</i> ,13 <i>R</i> ,15 <i>R</i> ,16 <i>S</i> ,18 <i>R</i> ,20 <i>R</i> ,21 <i>S</i> ,23 <i>R</i> ,25 <i>R</i> ,26 <i>S</i> ,28 <i>R</i> ,30 <i>R</i> ,31 <i>S</i> ,33 <i>R</i> ,35 <i>R</i> ,36 <i>R</i> ,37 <i>R</i> ,38 <i>R</i> ,39 <i>R</i> ,40 <i>R</i> ,41 <i>R</i> ,42 <i>R</i> ,43 <i>R</i> ,44 <i>R</i> ,45 <i>R</i> ,46 <i>R</i> ,47 <i>R</i> ,48 <i>R</i> ,49 <i>R</i>)-36,37,38,39,40,41,42,43,44,45,46,47,48,49-tetradecahydroxy-5,15,20,25,30,35-Hexakis(hydroxymethyl)-2,4,7,9,12,14,17,19,22,24,27,29,32,34-tetradeca-octa-cyclo[31.2.2.23.6.28,11.213,16.218,21.223,26.228,31]nonatetracontan-10-yl]methyl 4-methylbenzenesulfonate
InChI	InChI=1S/C49H76O37S/c1-13-2-4-14(5-3-13)87(70,71)72-12-21-42-28(62)35(69)49(79-21)85-41-20(11-55)77-47(33(67)26(41)60)83-39-18(9-53)75-45(31(65)24(39)58)81-37-16(7-51)73-43(29(63)22(37)56)80-36-15(6-50)74-44(30(64)23(36)57)82-38-17(8-52)76-46(32(66)25(38)59)84-40-19(10-54)78-48(86-42)34(68)27(40)61/h2-5,15-69H,6-12H2,1H3/t15-,16-,17-,18-,19-,20-,21-,22-,23-,24-,25-,26-,27-,28-,29-,30-,31-,32-,33-,34-,35-,36-,37-,38-,39-,40-,41-,42-,43-,44-,45-,46-,47-,48-,49-/m1/s1
InChI Key	URYLJCBFCXEADB-XISQNVKBSA-N
Canonical SMILES	CC1=CC=C(C=C1)S(=O)(=O)OCC2C3C(C(C(O2)OC4C(OC(C(C4O)O)OC5C(OC(C(C5O)O)OC6C(OC(C(C6O)O)OC7C(OC(C(C7O)O)OC8C(OC(C(C8O)O)OC9C(OC(O3)C(C9O)O)CO)CO)CO)CO)CO)O)O
Isomeric SMILES	CC1=CC=C(C=C1)S(=O)(=O)OC[C@@H]2[C@@H]3[C@@H]([C@H]([C@H](O2)O[C@@H]4[C@@H](O[C@@H]([C@@H]([C@H]4O)O)O[C@@H]5[C@H](O[C@@H]([C@@H]([C@H]5O)O)O[C@@H]6[C@H](O[C@@H]([C@@H]([C@H]6O)O)O[C@@H]7[C@H](O[C@@H]([C@@H]([C@H]7O)O)O[C@@H]8[C@H](O[C@@H]([C@@H]([C@H]8O)O)O[C@@H]9[C@H](O[C@H](O3)[C@@H]([C@@H]9O)O)CO)CO)CO)CO)CO)O)O
Form	White to slight yellow powder
Purity	>97%
Impurities	Beta-cyclodextrin
Solubility	6-Mono-O-(<i>p</i> -toluenesulfonyl)- β -cyclodextrin is soluble in DMF at 25°C.



Quality Level	Fine chemical grade
Applications	6-Mono- <i>O</i> -(<i>p</i> -toluenesulfonyl)- β -cyclodextrin is a monosubstituted cyclodextrin and can be used as a metal chelator that binds to metals.
Storage	Store at room temperature, in tightly closed container.
