



Product Information

Octakis(6-deoxy-6-bromo)- γ -cyclodextrin, Fine chemical grade

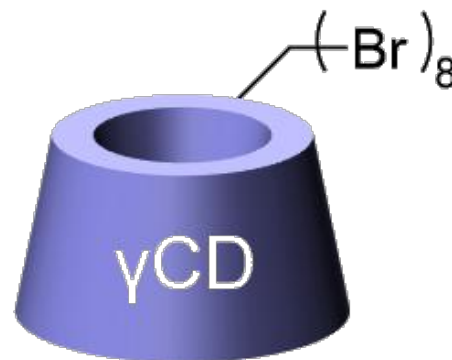
Cat. No.: X23-11-YM110

Size: 1 g; 5 g; 10 g; 50 g

CAS Number: 53784-84-2

Synonym: OBrGCD

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



Product Information

Molecular Weight	1800.3
Molecular Formula	C ₄₈ H ₇₂ O ₃₂ Br ₈
IUPAC Name	(1S,3S,5S,6S,8S,10S,11S,13S,15S,16S,18S,20S,21S,23S,25S,26S,28S,30S,31S,33S,35S,36S,38S,40S,41R,42R,43R,44R,45R,46R,47R,48R,49R,50R,51R,52R,53R,54R,55R,56R)-5,10,15,20,25,30,35,40-Octakis(bromomethyl)-2,4,7,9,12,14,17,19,22,24,27,29,32,34,37,39-hexadecaioxanonacyclo[36.2.2.23.6.28,11.213,16.218,21.223,26.228,31.233,36]hexapentacontane-41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56-hexadecol
InChI	InChI=1S/C48H72Br8O32/c49-1-9-33-17(57)25(65)41(73-9)82-34-10(2-50)75-43(27(67)19(34)59)84-36-12(4-52)77-45(29(69)21(36)61)86-38-14(6-54)79-47(31(71)23(38)63)88-40-16(8-56)80-48(32(72)24(40)64)87-39-15(7-55)78-46(30(70)22(39)62)85-37-13(5-53)76-44(28(68)20(37)60)83-35-11(3-51)74-42(81-33)26(66)18(35)58/h9-48,57-72H,1-8H2/t9-,10-,11-,12-,13-,14-,15-,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-/m1/s1
InChI Key	ONWAJCGYJSVQSX-HSEONFRVSA-N
Canonical SMILES	C(C1C2C(C(C(O1)OC3C(OC(C(C3O)O)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(O2)C(C9O)O)CBr)CBr)CBr)CBr)CBr)CBr)CBr)O)O)Br
Isomeric SMILES	C([C@@H]1[C@@H]2[C@@H]([C@H]([C@H](O1)O[C@@H]3[C@H](O[C@@H]([C@@H]([C@H]3O)O)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](O2)[C@@H]([C@H]9O)O)CBr)CBr)CBr)CBr)CBr)CBr)O)O)Br
Form	White to slight yellow powder
Purity	>90%



Impurities	Gamma-cyclodextrin, over- and underbrominated gamma-cyclodextrins, triphenylphosphine related substances
Solubility	Octakis(6-deoxy-6-bromo)- γ -cyclodextrin is soluble in DMF, but insoluble in methanol and water at 25°C.
Quality Level	Fine chemical grade
Applications	Octakis(6-deoxy-6-bromo)- γ -cyclodextrin is a single isomer, and can be used in the development of new materials, catalysts, and molecular recognition systems.
Storage	Store at room temperature, in tightly closed container.
