(1S,3R,5R,6S,8R,10R,11S,13R,15R,16S,18R,20R,21S,23R,25R,26S,28R,30R,31R,32R,33R,34R,35R,36R,37R,38R,39R,40R,41R,42R)-5,10,15,20,25,30-HEXAKIS(HYDROXYMETHYL)-2,4,7,9,12,14,17,19,22,24,27,29-DODECAOXAHEPTACYCLO[26.2.2.2^{3,6}.2^{8,11}.2^{13,16}.2^{18,21}.2^{23,26}]DOTETRACONTANE-31,32,33,34,35,36,37,38,39,40,41,42-DODECOL
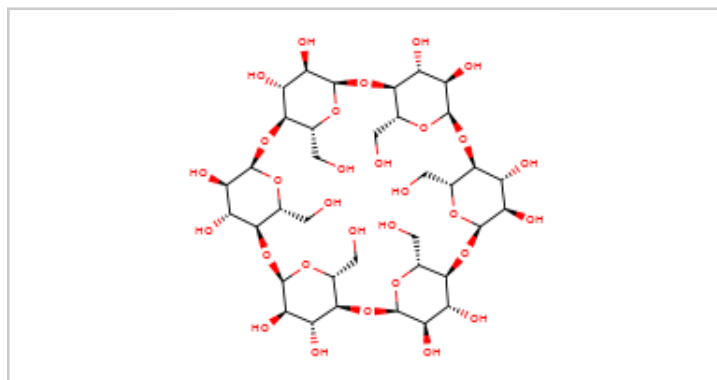
Catalog Id:

MM10016203

IUPAC:

A-CYCLODEXTRIN

CAS Number:

10016-20-3

More Information:

Molecular Weight: 972.846

Formula: $C_{36}H_{60}O_{30}$

SMILES:

OC[C@H]1O[C@@H]2O[C@@H]3[C@@H](CO)O[C@H](O[C@@H]4[C@@H](CO)O[C@H](O[C@@H]5[C@@H](CO)O[C@H](O[C@@H]6[C@@

Preferred IUPAC Name:

(1S,3R,5R,6S,8R,10R,11S,13R,15R,16S,18R,20R,21S,23R,25R,26S,28R,30R,31R,32R,33R,34R,35R,36R,37R,38R,39R,40R,41R,42R)-5,10,15,20,25,30-HEXAKIS(HYDROXYMETHYL)-2,4,7,9,12,14,17,19,22,24,27,29-DODECAOXAHEPTACYCLO[26.2.2.2^{3,6}.2^{8,11}.2^{13,16}.2^{18,21}.2^{23,26}]DOTETRACONTANE-31,32,33,34,35,36,37,38,39,40,41,42-DODECOL

InChIKey: InChIKey=HFHDHCJBZVLPGP-RWMJIURBSA-N