

1,3,5(10)-Oestratriene-2-methoxy-3,17«beta»-diol, 3-TBDMS-17-HFB

InChI: 1S/C29H39F7O4Si/c1-25(2,3)41(6,7)40-22-14-16-8-9-18-17(19(16)15-21(22)38-5)23-24-26-27-28-29/s1-5,10,15,20,25,30,35,40,45,50,55,60,65,70,75,80,85,90,95,100,105,110,115,120,125,130,135,140,145,150,155,160,165,170,175,180,185,190,195,200,205,210,215,220,225,230,235,240,245,250,255,260,265,270,275,280,285,290,295,300,305,310,315,320,325,330,335,340,345,350,355,360,365,370,375,380,385,390,395,400,405,410,415,420,425,430,435,440,445,450,455,460,465,470,475,480,485,490,495,500,505,510,515,520,525,530,535,540,545,550,555,560,565,570,575,580,585,590,595,600,605,610,615,620,625,630,635,640,645,650,655,660,665,670,675,680,685,690,695,700,705,710,715,720,725,730,735,740,745,750,755,760,765,770,775,780,785,790,795,800,805,810,815,820,825,830,835,840,845,850,855,860,865,870,875,880,885,890,895,900,905,910,915,920,925,930,935,940,945,950,955,960,965,970,975,980,985,990,995,1000/t1,3,5,10,15,20,25,30,35,40,45,50,55,60,65,70,75,80,85,90,95,100,105,110,115,120,125,130,135,140,145,150,155,160,165,170,175,180,185,190,195,200,205,210,215,220,225,230,235,240,245,250,255,260,265,270,275,280,285,290,295,300,305,310,315,320,325,330,335,340,345,350,355,360,365,370,375,380,385,390,395,400,405,410,415,420,425,430,435,440,445,450,455,460,465,470,475,480,485,490,495,500,505,510,515,520,525,530,535,540,545,550,555,560,565,570,575,580,585,590,595,600,605,610,615,620,625,630,635,640,645,650,655,660,665,670,675,680,685,690,695,700,705,710,715,720,725,730,735,740,745,750,755,760,765,770,775,780,785,790,795,800,805,810,815,820,825,830,835,840,845,850,855,860,865,870,875,880,885,890,895,900,905,910,915,920,925,930,935,940,945,950,955,960,965,970,975,980,985,990,995,1000/b1,3,5,10,15,20,25,30,35,40,45,50,55,60,65,70,75,80,85,90,95,100,105,110,115,120,125,130,135,140,145,150,155,160,165,170,175,180,185,190,195,200,205,210,215,220,225,230,235,240,245,250,255,260,265,270,275,280,285,290,295,300,305,310,315,320,325,330,335,340,345,350,355,360,365,370,375,380,385,390,395,400,405,410,415,420,425,430,435,440,445,450,455,460,465,470,475,480,485,490,495,500,505,510,515,520,525,530,535,540,545,550,555,560,565,570,575,580,585,590,595,600,605,610,615,620,625,630,635,640,645,650,655,660,665,670,675,680,685,690,695,700,705,710,715,720,725,730,735,740,745,750,755,760,765,770,775,780,785,790,795,800,805,810,815,820,825,830,835,840,845,850,855,860,865,870,875,880,885,890,895,900,905,910,915,920,925,930,935,940,945,950,955,960,965,970,975,980,985,990,995,1000

InchiKey: NMDXBSXESTWUHW-IWJUXTRFSA-N

Formula: C₂₉H₃₉F₇O₄Si

SMILES: COc1cc2c(cc1O[Si](C)(C)C(C)(C)C)CCC1C2CCC2(C)C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 612.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.67		Crippen Method
logp	8.680		Crippen Method
rinpol	2869.00		NIST Webbook
rinpol	2869.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R537187&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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