trans-Dehydroandrosterone, picolinyloxydimethylsilyl ether

Inchi: InChI=1S/C27H39NO3Si/c1-26-13-11-21(31-32(3,4)30-18-19-6-5-15-28-17-19)16-20(26)7-8-22-23-9-10-25(29)27(23,2)14-12-24(22)26/h5-6,15,17,20-24H,7-14,16,18H2,1-4H3/t20-,21-,22-,23-,24-,26-,27-/m0/s1

InchiKey: CHLYURRBCUAVER-UHFFFAOYSA-N

Formula: C27H39NO3Si

SMILES: CC12CCC3C(CC=C4CC(O[Si](C)(C)OCc5cccnc5)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 453.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.33		Crippen Method
logp	6.217		Crippen Method
rinpol	3520.80		NIST Webbook
rinpol	3520.80		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U352249&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices