11-Hydroxyetiocholanolone MO TMS

Other names: 11-«beta»-Hydroxyetiocholanolone, MO TMS
11B-Hydroxyetiocholanolone, MO TMS
Inchi: InChI=1S/C26H49NO3Si2/c1-25-15-14-19(29-31(4,5)6)16-18(25)10-11-20-21-12-13-23(2
InchiKey: XCNGMXKDGCALRD-DJBVTNEDSA-N
Formula: C26H49NO3Si2
SMILES: CON=C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12C
Mol. weight [g/mol]: 479.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	7.082		Crippen Method
rinpol	2709.00		NIST Webbook
rinpol	2721.00		NIST Webbook
rinpol	2744.00		NIST Webbook
rinpol	2723.00		NIST Webbook
rinpol	2700.00		NIST Webbook
rinpol	2712.00		NIST Webbook
rinpol	2734.00		NIST Webbook
rinpol	2732.00		NIST Webbook
rinpol	2712.00		NIST Webbook
rinpol	2737.00		NIST Webbook
rinpol	2723.00		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=R92719&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices