11-Ketoetiocholanolone MO TMS

Other names: 11-oxoetiocholanolone, MO TMS
Inchi: InChI=1S/C24H42N2O3Si/c1-23-13-12-17(29-30(5,6)7)14-16(23)8-9-18-19-10-11-21(26-
InchiKey: CZAVIQKBQLKTIH-OUBBBTIISA-N
Formula: C24H42N2O3Si
SMILES: CON=C1CC2(C)C(=NOC)CCC2C2CCC3CC(O[Si](C)(C)C)CCC3(C)C12
Mol. weight [g/mol]: 434.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Crippen Method
logp	5.864		Crippen Method
rinpol	2627.00		NIST Webbook
rinpol	2630.00		NIST Webbook
rinpol	2610.00		NIST Webbook
rinpol	2632.00		NIST Webbook
rinpol	2636.00		NIST Webbook
rinpol	2656.00		NIST Webbook
rinpol	2646.00		NIST Webbook
rinpol	2601.00		NIST Webbook
rinpol	2601.00		NIST Webbook
rinpol	2627.00		NIST Webbook
rinpol	2610.00		NIST Webbook
rinpol	2656.00		NIST Webbook
rinpol	2610.00		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=R92666&Units=SI

Legend

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