5-Pregnen-3«beta»-ol-20-one, MO-TMS

Inchi: InChI=1S/C25H43NO2Si/c1-17(26-27-4)21-10-11-22-20-9-8-18-16-19(28-29(5,6)7)12-14
InchiKey: UJRFOJLCOGKWOK-CRHFWZTASA-N
Formula: C25H43NO2Si
SMILES: CON=C(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 417.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	6.808		Crippen Method
rinpol	2759.00		NIST Webbook
rinpol	2728.00		NIST Webbook
rinpol	2759.00		NIST Webbook
rinpol	2728.00		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=R487235&Units=SI

Legend

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