Practolol, TBDMS

Inchi:	InChI=1S/C26H50N2O3Si2/c1-20(2)27-18-24(31-33(12,13)26(7,8)9)19-29-23-16-14-22(1
InchiKey:	PGHAFSDYRXUHOY-HFTWOUSFSA-N
Formula:	C26H50N2O3Si2
SMILES:	CC(=Nc1ccc(OCC(CNC(C)C)O[Si](C)(C)C(C)(C)C)cc1)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	494.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	7.525		Crippen Method
rinpol	2695.10		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=R435308&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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