Propranolol tbdms

Other names: Propranolol, tbdms derivative
Inchi: InChI=1S/C22H35NO2Si/c1-17(2)23-15-19(25-26(6,7)22(3,4)5)16-24-21-14-10-12-18-11
InchiKey: WACGWDSOXLNZOE-UHFFFAOYSA-N
Formula: C22H35NO2Si
SMILES: CC(C)NCC(COc1cccc2ccccc12)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 373.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Crippen Method
logp	5.607		Crippen Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		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=U331808&Units=SI

Legend

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