Penbutolol, TBDMS

Inchi: InChI=1S/C24H43NO2Si/c1-23(2,3)25-17-20(27-28(7,8)24(4,5)6)18-26-22-16-12-11-15-2
InchiKey: MSACJEKWZUAOJV-UHFFFAOYSA-N
Formula: C24H43NO2Si
SMILES: CC(C)(C)NCC(COc1ccccc1C1CCCC1)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 405.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	6.502		Crippen Method
rinpol	2351.10		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R435264&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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