Synephryne, N-isoBOC, O-TBDMS

Inchi: InChI=1S/C26H49NO4Si2/c1-20(2)19-29-24(28)27(9)18-23(31-33(12,13)26(6,7)8)21-14-
InchiKey: XTNSJBGYKYZJPJ-UHFFFAOYSA-N
Formula: C26H49NO4Si2
SMILES: CC(C)COC(=O)N(C)CC(O[Si](C)(C)C(C)(C)C)c1ccc(O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]: 495.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	7.858		Crippen Method
rinpol	2771.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R392855&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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