Rhodoporphyrin-XV homologue, bis(trimethylsiloxy)silicon(IV) derivative

Inchi: InChI=1S/C38H50N4O4Si2/c1-13-25-21(3)28-17-29-23(5)27(15-16-36(43)45-47(7,8)9)34

InchiKey: DSGDICSAKPOVTF-PFEKHQJSSA-N

Formula: C38H50N4O4Si2

SMILES: CCC1=C(C)c2cc3nc(cc4[nH]c(cc5[nH]c(cc1n2)c(C)c5CC)c(C)c4C(=O)O[Si](C)(C)C)C(C

Mol. weight [g/mol]: 683.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.08		Crippen Method
logp	8.952		Crippen Method
rinpol	3905.00		NIST Webbook
rinpol	3905.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R149394&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