Aetioporphyrin-I, bis(trimethylsiloxy)silicon(IV) derivative

Inchi: InChI=1S/C38H54N4Si2/c1-15-27-24(6)32-20-37-29(17-3)26(8)36(42(37)44(12,13)14)22

InchiKey: KIBGMUHJXJNUAG-JQRPMTNOSA-N

Formula: C38H54N4Si2

SMILES: CCC1=C(C)c2cc3c(CC)c(C)c(cc4c(CC)c(C)c(cc5nc(cc1n2)C(C)=C5CC)n4[Si](C)(C)C)n3

Mol. weight [g/mol]: 623.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.40		Crippen Method
logp	11.051		Crippen Method
rinpol	3330.00		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=R149354&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices