C31-Aetio-porphyrin, Si-(OTMS)2-derivative

Inchi: InChI=1S/C37H52N4O2Si3/c1-15-27-24(6)30-18-34-22(4)23(5)35-20-32-28(16-2)25(7)31
InchiKey: ABUGPPZUQKANIA-XGRMMTBOSA-N
Formula: C37H52N4O2Si3
SMILES: CCC1=C(C)C2=NC1=Cc1c(C)c(C)c3n1[Si](O[Si](C)(C)C)(O[Si](C)(C)C)n1c(c(C)c(CC)c1
Mol. weight [g/mol]: 669.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.73		Crippen Method
logp	7.944		Crippen Method
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R530780&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