Mesoporphyrin-IX dimethyl ester, bis(trimethylsiloxy)silicon(IV) derivative

Inchi: InChI=1S/C42H58N4O4Si2/c1-15-29-25(3)34-22-37-27(5)30(16-2)40(45(37)51(9,10)11)2

InchiKey: LPLZPTBJNMWOAI-IWQYSSHZSA-N

Formula: C42H58N4O4Si2

SMILES: CCC1=C(C)c2cc3c(C)c(CC)c(cc4c(C)c(CCC(=O)OC)c(cc5nc(cc1n2)C(C)=C5CCC(=O)O

Mol. weight [g/mol]: 739.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.80		Crippen Method
logp	10.137		Crippen Method
rinpol	3975.00		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=R149374&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices