Silica-octaethylporphyrine complex, bis-OTBDMS

Inchi: InChI=1S/C48H76N4O2Si3/c1-19-31-32(20-2)40-28-44-37(25-7)38(26-8)46-30-42-34(22

InchiKey: LAUBRJUKBZZCBE-AQXATVBXSA-N

Formula: C48H76N4O2Si3

SMILES: CCc1c2[nH]c(c1CC)C=c1c(CC)c(CC)c3n1[Si](O[Si](C)(C)C(C)(C)C)(O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 825.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.42		Crippen Method
logp	8.299		Crippen Method
rinpol	3835.00		NIST Webbook
rinpol	3835.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R388202&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