Octaethyl-porphyrin, Si-(OTBDMS)2-derivative

Inchi:	InChI=1S/C48H74N4O2Si3/c1-19-31-32(20-2)40-28-44-37(25-7)38(26-8)46-30-42-34(22
InchiKey:	DEMVBRZYNLPFAO-AQXATVBXSA-N
Formula:	C48H74N4O2Si3
SMILES:	CCC1=C(CC)C2=NC1=Cc1c(CC)c(CC)c3n1[Si](O[Si](C)(C)C(C)(C)C)(O[Si](C)(C)C(C)(C
Mol. weight [g/mol]:	823.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.06		Crippen Method
logp	11.827		Crippen Method
rinpol	3835.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R530859&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

Latest version available from:
https://www.chemeo.com/cid/22-426-4/Octaethyl-porphyrin-Si-OTBDMS-2-derivative.pdf
Generated by Cheméo on 2024-04-19 22:08:05.755178997 +0000 UTC m=+15853734.675756319.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.