

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(22-2)
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
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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/ci9903071

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/71-067-9/Silica-octaethylporphyrine-complex-bis-OTBDMS.pdf>

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