

Silica-1,3,5,7,8-pentamethyl-2,4,6-triethylporphyrine complex, bis-OTMS

InChI: InChI=1S C37H54N4O2Si3/c1-15-27-24(6)30-18-34-22(4)23(5)35-20-32-28(16-2)25(7)3
InChIKey: RGSGHBLWKLLAPI-XGRMMTBOSA-N

Formula: C37H54N4O2Si3

SMILES: CCc1c2[nH]c(c1C)C=c1c(CC)c(C)c3n1[Si](O[Si](C)(C)C)(O[Si](C)(C)C)n1c(c(C)c(C)c1=C

Mol. weight [g/mol]: 671.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	4.688		Crippen Method
rinpol	3300.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R388168&Units=SI>

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/71-030-9/Silica-1-3-5-7-8-pentamethyl-2-4-6-triethylporphyrine-complex-bis-OTMS.pdf>

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