

Silica-octamethylporphyrine complex, bis-OTMS

Inchi:	InChI=1S/C34H48N4O2Si3/c1-19-20(2)28-16-32-25(7)26(8)34-18-30-22(4)21(3)29(36-3
InchiKey:	OQQNEVKISXVESL-YLPLBUAGSA-N
Formula:	C34H48N4O2Si3
SMILES:	Cc1c2[nH]c(c1C)C=c1c(C)c(C)c3n1[Si](O[Si](C)(C)C)(O[Si](C)(C)C)n1c(c(C)c(C)c1=Cc1
Mol. weight [g/mol]:	629.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Crippen Method
logp	3.926		Crippen Method
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R388222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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.cheméo.com/cid/49-165-5/Silica-octamethylporphyrine-complex-bis-OTMS.pdf>

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