

Rhodoporphyrin-XV homologue, bis(trimethylsiloxy)silicon(IV) derivative

Inchi: InChI=1S/C38H50N4O4Si2/c1-13-25-21(3)28-17-29-23(5)27(15-16-36(43)45-47(7,8)9)34
InchiKey: DSGDICSAPOVTF-PFEKHQJSSA-N
Formula: C38H50N4O4Si2
SMILES: CCC1=C(C)c2cc3nc(cc4[nH]c(cc5[nH]c(cc1n2)c(C)c5CC)c(C)c4C(=O)O[Si](C)(C)C)C(C)C
Mol. weight [g/mol]: 683.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.08		Crippen Method
logp	8.952		Crippen Method
rinpol	3905.00		NIST Webbook
rinpol	3905.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R149394&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/119-019-9/Rhodoporphyrin-XV-homologue-bis-trimethylsiloxy-silicon-IV-derivative.pdf>

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