

# Deuteroporphyrin-IX dimethyl ester, bis(trimethylsiloxy)silicon(IV) derivative

**Inchi:** InChI=1S/C38H50N4O4Si2/c1-23-17-27-19-32-25(3)29(13-15-37(43)45-5)33(40-32)21-3  
**InchiKey:** WRAJCWQFWYBLPA-GQCZFTIJSJSA-N  
**Formula:** C38H50N4O4Si2  
**SMILES:** COC(=O)CCC1=C(C)c2cc3nc(cc4cc(C)c(cc5c(C)c(CCC(=O)OC)c(cc1n2)n5[Si](C)(C)C)n

**Mol. weight [g/mol]:** 683.00

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.16		Crippen Method
logp	8.794		Crippen Method
rinpol	3850.00		NIST Webbook
rinpol	3850.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R149369&Units=SI>

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

**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](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

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