

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

Inchi: InChI=1S/C42H58N4O4Si2/c1-15-29-25(3)34-22-37-27(5)30(16-2)40(45(37)51(9,10)11)2
InchiKey: LPLZPTBJNMWOAI-IWQYSSHZSA-N
Formula: C42H58N4O4Si2
SMILES: CCC1=C(C)c2cc3c(C)c(CC)c(cc4c(C)c(CCC(=O)OC)c(cc5nc(cc1n2)C(C)=C5CCC(=O)O)C)C
Mol. weight [g/mol]: 739.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.80		Crippen Method
logp	10.137		Crippen Method
rinpol	3975.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R149374&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.cheméo.com/cid/40-768-5/Mesoporphyrin-IX-dimethyl-ester-bis-trimethylsiloxy-silicon-IV-derivative.pdf>

Generated by Cheméo on 2024-05-01 00:23:28.84376609 +0000 UTC m=+16812257.764343405.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.