d4-Cystine, tri-TMS

Inchi: InChI=1S/C15H36N2O4S2Si3/c1-24(2,3)17-13(15(19)21-26(7,8)9)11-23-22-10-12(16)14

InchiKey: NIRWUGJVFWNGAW-MKQHWYKPSA-N

Formula: C15H32D4N2O4S2Si3

SMILES: C[Si](C)(C)NC(CSSCC(N)C(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 460.87

Physical Properties

Property code	Value	Unit	Source
log10ws	2.42		Crippen Method
logp	3.244		Crippen Method
rinpol	2319.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R330179&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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