Homo-cystine, TMS

Inchi: InChI=1S/C20H48N2O4S2Si4/c1-29(2,3)21-17(19(23)25-31(7,8)9)13-15-27-28-16-14-18
InchiKey: VVODJOVRLCDBOE-UHFFFAOYSA-N
Formula: C20H48N2O4S2Si4
SMILES: C[Si](C)(C)NC(CCSSCCC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 557.08

Physical Properties

Property code	Value	Unit	Source
log10ws	2.52		Crippen Method
logp	5.490		Crippen Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R305410&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices