1-Kestose, TMS

Inchi: InChI=1S/C51H120O16Si11/c1-68(2,3)53-34-39-42(61-72(13,14)15)45(64-75(22,23)24)4
InchiKey: SWHJUYJGRRIDPF-DOJLZCONSA-N
Formula: C51H120O16Si11
SMILES: C[Si](C)(C)OCC1OC(OC2(COC3(CO[Si](C)(C)C)OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C3C
Mol. weight [g/mol]: 1298.43

Physical Properties

Property code	Value	Unit	Source
log10ws	12.25		Crippen Method
logp	12.881		Crippen Method
rinpol	3360.00		NIST Webbook
rinpol	3360.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R614378&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