O-Methyl-scyllo-inositol, pentakis-TMS

Inchi: InChI=1S/C22H54O6Si5/c1-23-17-18(24-29(2,3)4)20(26-31(8,9)10)22(28-33(14,15)16)21
InchiKey: IKOVCQNLJNHSBD-RGHYKDJOSA-N
Formula: C22H54O6Si5
SMILES: COC1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 555.09

Physical Properties

Property code	Value	Unit	Source
log10ws	5.62		Crippen Method
logp	6.115		Crippen Method
rinpol	2025.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	2025.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R532028&Units=SI

Legend

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