Sorbitol, 2-methyl, TMS

Inchi: InChI=1S/C22H56O6Si5/c1-23-19(17-24-29(2,3)4)21(27-32(11,12)13)22(28-33(14,15)16
InchiKey: RSBYKFAKZCZKRL-LRSLUSHPSA-N
Formula: C22H56O6Si5
SMILES: COC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 557.10

Physical Properties

Property code	Value	Unit	Source
log10ws	5.74		Crippen Method
logp	6.365		Crippen Method
rinpol	1790.00		NIST Webbook
rinpol	1786.00		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=R527749&Units=SI

Legend

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