D-Pinitol, TMS

Other names: D(+)-Pinitol, 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-MCSHHISBSA-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	1880.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1869.00		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=R441353&Units=SI

Legend

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