Rhamnitol, TMS

Inchi: InChI=1S/C21H54O5Si5/c1-18(23-28(5,6)7)20(25-30(11,12)13)21(26-31(14,15)16)19(24
InchiKey: YCLDNNFGQOEZPF-ANULTFPQSA-N
Formula: C21H54O5Si5
SMILES: CC(O[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]: 527.08

Physical Properties

Property code	Value	Unit	Source
log10ws	5.25		Crippen Method
logp	6.738		Crippen Method
rinpol	1817.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R7095&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