cellobutol, TMS

Inchi: InChI=1S/C40H98O11Si9/c1-52(2,3)31-42-32(35(47-56(13,14)15)37(49-58(19,20)21)34(
InchiKey: VHQIBTOGUDBOSM-LUFYFMEXSA-N
Formula: C40H98O11Si9
SMILES: C[Si](C)(C)COC(COC1OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)
Mol. weight [g/mol]: 1007.97

Physical Properties

Property code	Value	Unit	Source
log10ws	10.11		Crippen Method
logp	11.014		Crippen Method
rinpol	2903.20		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R488892&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