«alpha»-Neolactose, TMS

Inchi: InChI=1S/C36H86O11Si8/c1-48(2,3)37-25-27-30(43-51(10,11)12)32(45-53(16,17)18)34(
InchiKey: BKRCJVHGUNBEML-VJTRPLOFSA-N
Formula: C36H86O11Si8
SMILES: C[Si](C)(C)OCC1OC(O[Si](C)(C)C)C(OC2OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(
Mol. weight [g/mol]: 919.75

Physical Properties

Property code	Value	Unit	Source
log10ws	8.84		Crippen Method
logp	9.476		Crippen Method
rinpol	2671.00		NIST Webbook
rinpol	2671.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R67926&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