«alpha»-Melibiose TMS

Inchi: InChI=1S/C36H86O11Si8/c1-48(2,3)38-26-28-30(42-50(7,8)9)31(43-51(10,11)12)33(45-5
InchiKey: SWPQHIFGBMZXPV-PWNVFHPSSA-N
Formula: C36H86O11Si8
SMILES: C[Si](C)(C)OCC1OC(OCC2OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C2O[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	2924.00		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=R24574&Units=SI

Legend

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