«alpha»,«alpha»-trehalose, TMS

Inchi: InChI=1S/C36H86O11Si8/c1-48(2,3)37-25-27-29(42-50(7,8)9)31(44-52(13,14)15)33(46-5

InchiKey: YQFZNYCPHIXROS-FSZCTWQYSA-N

Formula: C36H86O11Si8

SMILES: C[Si](C)(C)OCC1OC(OC2OC(CO[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
logp	9.476		Crippen Method
rinpol	2850.10		NIST Webbook
rinpol	2816.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R488812&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices